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James A. Thomas, Jr.

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*This work was completed while the author was a graduate student in the Theoretical Chemistry Institute of the University of Wisconsin.

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THE TRANSPORT PROPERTIES OF DILUTE GASES IN APPLIED FIELDS*

James A. Thomas, Jr.

Under the supervision of Professor C. F. Curtiss

ABSTRACT

Collision integrals developed and partially evaluated by L. W. Hunter and R. F. Snider, and utilized by Hunter in his treatment of the effects of a magnetic field on the shear viscosity and thermal conductivity of single component diatomic gases, are cast in the Generalized Phase Shift (GPS) formalism of C. F. Curtiss. This, along with the introduction of certain operators, allows the collision integrals to be considerably simplified by facilitating the evaluation of several summations and angle integrations.

The difficulties inherent in treating diatom-diatom interactions lead to consideration of binary gaseous mixtures in which the dominant species is atomic, the diatomic species being restricted to low concentrations. Such systems require consideration of atom-atom and atom-diatom interactions only. Employing methods introduced by Hunter, scalar equations are obtained for the transport properties of binary mixtures in applied magnetic fields. The collision integrals occurring in

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these equations are found to be generalizations of those discussed by Hunter and Snider.

The shear viscosity of an atom-diatom mixture in an applied magnetic field is then treated in detail. The basis set is truncated and the diatomic species is restricted to low concentrations. The expressions obtained for the shear viscosity tensor are in qualitative agreement with experimental observations. Steps leading to calculation of the shear viscosity tensor in this particular case are discussed.

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INTRODUCTION

1. The Senftleben-Beenakker Effect

Calculated values of the transport properties of dilute polyatomic gases that compare favorably with experimentally measured values can be obtained[1] by treating the molecules as point particles, i.e., as structureless particles interacting via a spherical intermolecular potential. Incorporating internal molecular structure and angular dependence of the interaction potential complicates the transport property calculations considerably, but makes only small contributions to the calculated value. This fact somewhat reduces the incentive for carrying out such calculations, and makes it difficult to assess the relative merits of various treatments of the non-spherical contribution. The spherical treatment, however, is incapable of accounting for the effect of an applied external field on the transport properties of polyatomic molecules. This effect, known as the Senftleben-Beenakker effect for the men who first observed it experimentally for paramagnetic and diamagnetic molecules, respectively, can actually be measured more accurately than the transport properties themselves.[2] It is extremely sensitive to the anisotropic part of the intermolecular potential of molecules possessing internal structure, and for this reason, may provide a useful means of probing nonspherical interactions.

There is a simple physical explanation[3] of the effect. Under the influence of a gradient in one or more of the macroscopic variables of a system, the molecules tend to change their distribution so as to reduce the magnitude of the gradient, or gradients involved. The result is a flow within the system. Since the molecules are nonspherical, the collision probabilities are functions of the orientations, and consequently, the molecules have a tendency to align. This results in a value for the transport property that is slightly larger than that which would obtain in the absence of any alignment.

Since both paramagnetic and diamagnetic molecules have net magnetic moments, in the presence of a magnetic field they precess about the field direction. Except for those components parallel to the field, this precession tends to destroy the preferential alignments, or polarizations, resulting from the presence of the gradients. As a consequence, the transport properties of molecules with net magnetic moments are reduced[4] in the presence of an external magnetic field.

The extent of the destruction of the polarizations is directly related to the average number of precessions between collisions. The precession frequency is proportional to the magnetic field strength, H_M, while the time between collisions is inversely proportional to the pressure, p, for a dilute

gas. At constant temperature, the extent of the destruction of polarization, and consequently the Senftleben-Beenakker effect, is solely a function of H_{μ}/p . At sufficiently high field strengths, polarization is completely destroyed, and saturation occurs.

In extending the above picture, it is apparent that any polyatomic gas will exhibit a similar effect when subjected to an external field capable of causing the molecules to precess. Other than the case of polar molecules in electric fields, however, the field strengths required to cause a reasonable degree of precession are so high as to make practical applications virtually impossible.[4]

2. Theory and Experiment – A Brief History[4,5]

The effect of a magnetic field on the thermal conductivity of gaseous O_2 was first observed by H. Senftleben[6] in 1930. Engelhardt and Sack[7] then observed the Senftleben effect on the viscosity of O_2 in 1932. The fact that NO behaves in the same manner as O_2 coupled with the fact that in mixtures with non-paramagnetic gases, the effect is proportional to the mole fraction of the paramagnetic species, led early observers to the (erroneous) conclusion that the Senftleben effect is a property of paramagnetic gases only. Other observations of the first decade[4] of such studies were that in the presence of a magnetic field, the transport coefficients of paramagnetic gases decrease by from 0.1 to 1.0%; that the effect is even in the magnetic field; and that at constant temperature, it is a function of the field strength divided by the pressure.

The observations of the first decade led C. J. Gorter[8] to an early qualitative explanation of the effect in 1938. His explanation, based upon consideration of the effect of a magnetic field on the mean free path of an O_2 molecule, was treated more quantitatively in 1939 by Zernike and van Lier.[9] These early developments treated the rotating paramagnetic molecule as a disc with a magnetic moment in the direction of the axis of rotation. The cross section depends on the angle

between the axis of rotation and the direction of motion. In the absence of a magnetic field, the direction of the axis of rotation is conserved between collisions. In the presence of a field, however, the magnetic moment, and consequently the axis of rotation, precesses about the direction of the field. The collision cross section now changes periodically during the flight of the molecule, necessitating an averaging over the precessions in the mean-free-path picture. This additional averaging leads to the decrease in the transport properties. The mean-free-path approach adequately accounts for the phenomenon of saturation, the functional dependence on H_M/p, and the dependence on the mole fraction of paramagnetic species in a mixture.

Following the 1930's, during which the Senftleben effect on paramagnetic gases was studied extensively, essentially no studies of field effects took place until the early 1960's. Then in 1961, Kagan and Maksimov[10] presented a variational calculation of the Senftleben effect on the thermal conductivity of O_2. Their treatment of the linearized classical Boltzmann equation utilizes an elastic collision model and a truncated expansion of the distribution function in terms of irreducible Cartesian tensors in the (reduced peculiar) velocity, $\underline{W}$, and the rotational angular momentum, $\underline{J}$.

As early as 1939, Chapman and Cowling[11] had realized that in the presence of a perturbing gradient, for example $\underline{\nabla} \ln T$, the nonequilibrium distribution function, written as $f = f^{(0)}(1 + \phi)$ with $\phi = -\underline{A}\cdot\underline{\nabla} \ln T$, could contain terms involving $\underline{J}$. Since no physical reason was seen to consider polarization of nonspherical molecules in dilute gases at that time, they disregarded the anisotropy of the distribution function in $\underline{J}$, choosing instead to write $\underline{A}$ in the monatomic form, $A(W^2)\underline{W}$. In 1961, in a treatment of diatomics, Kagan and Afanas'ev[12] noted correctly that $\underline{A}$ should include terms involving all possible true vectors which can be constructed from $\underline{W}$ and $\underline{J}$, i.e., that $\underline{A}$ should be written as $\underline{A} = A_1\underline{W} + A_2\underline{W} \times \underline{J} + A_3(\underline{W}\cdot\underline{J})\underline{J}$. The Senftleben effect is then the result of the reduction of the anisotropy in $\underline{J}$ space due to the precession of the molecules in the presence of a magnetic field.

The following year, 1962, J. J. M. Beenakker[13] measured the change in the viscosity of N_2 and other diamagnetic gases in the presence of a magnetic field, removing the restriction of these field effects to paramagnetic molecules. Analogous measurements of the thermal conductivity were conducted by Gorelik and Sinitsyn[14] shortly thereafter. This experimental work involving field effects on diamagnetic gases has been followed by considerably renewed interest in the Senftleben-Beenakker effect from both experimental and theoretical standpoints.[5] Extensive

experimental information is now available, as well as numerous theoretical developments. Unfortunately, very few numerical calculations of field effects on transport properties have been attempted. This work is a step toward such calculations.

3. Scope

To date, most theoretical developments of the transport properties of polyatomic gases in applied fields utilize a Chapman-Enskog procedure[10] to solve the equations for the transport coefficients. Arguments are advanced to justify the truncations made, but most are not truly justified until the solution has been obtained.[2] L. W. Hunter has devised a procedure to treat transport properties that allows the tensor analysis to be completed before any truncation is necessary. Hunter's techniques are examined in Part I of this thesis, and the collision integrals arising in his treatment are cast in terms of the reduced scattering matrix of Curtiss[15] and co-workers. These collision integrals are then simplified considerably by the introduction of certain operators and the explicit evaluation of a number of the sums and angle integrals involved.

Hunter's treatment applies to a single-component diatomic gas. Calculation of the transport properties of such a system is complicated by the dependence of the interaction potential on the orientations of the colliding diatomics. Recently, a calculation of the transport properties of an atom-diatom mixture, in which the diatom is present in low concentration, has been completed by R. Wood.[16] Such a calculation requires consideration of atom-atom and atom-diatom interactions

exclusively. Since the Senftleben-Beenakker effect is observed in mixtures, it seems reasonable that a detailed calculation of the effect should first be attempted for an atom-diatom mixture involving a diamagnetic diatomic species in low concentration, and later generalized to a purely diatomic gas. In establishing the groundwork essential to an atom-diatom calculation, Hunter's development for a single component gas is first generalized to binary gas mixtures. This is accomplished in Part II.

Then in Part III, the equations derived in Part II for a binary gas mixture are restricted to an atom-diatom mixture that is predominantly atomic, and expressions for the shear viscosity are developed in detail. The expressions obtained are shown to be consistent with experimental results, and the collision integrals involved are expressed in such fashion as to make evident the extension of the calculations of R. Wood to the present problem.

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PART I

A SINGLE COMPONENT DIATOMIC GAS IN AN APPLIED MAGNETIC FIELD

I.1 Transport Coefficients

The linearized Waldmann-Snider equation[2,3] can be used to obtain a set of tensor equations from which the transport coefficients of a dilute gas can be determined. In most applications, the number of polarizations of the gas is limited to a finite set and the tensor analysis performed in a truncated basis. L. W. Hunter has developed a technique[1] for carrying out the tensor analysis with the complete set of polarizations, i.e. before truncation of the basis. In Reference 1, Hunter demonstrates this technique for the linear Zeeman effects on the shear viscosity and thermal conductivity of diamagnetic molecules. A sketch of Hunter's derivation of the scalar transport equations is given in this section. The analogous development for binary mixtures is carried out in detail in Part II.

In Hunter's work, the equations for the transport coefficients involve collision integrals which are related to those discussed and partially evaluated by Chen, Moraal, and Snider[4] and by

Hunter and Snider.[5] For convenience, expressions from Reference 1 will be referred to by their equation number (from the reference) preceded by H, e.g. H-40. Similarly, those from Reference 4 will be preceded by CMS, and those from Reference 5 by HS.

To obtain the basic tensor equations for the transport coefficients, the Wigner distribution function-density operator,[6] f , is expanded about the local equilibrium, $f^{(0)}$,

$$f = f^{(0)}(1 + \phi + \cdots). \qquad (I.1-1)$$

The perturbation, ϕ , is written in terms of quantities linear in gradients of the macroscopic variables. If only shear viscosity and thermal conductivity are of interest,[7]

$$\phi = -\underline{A}\cdot\underline{\nabla} \ln T - \underline{\underline{B}}:[\underline{\nabla}\underline{v}_0]^{(2)} , \qquad (I.1-2)$$

in which the bracket notation indicates a symmetric traceless tensor, T is the temperature, and $\underline{v}_0$ the stream velocity.

When (I.1-2) is used in the formal expressions for the heat flux, $\underline{q}$, and shear pressure tensor, $\underline{\underline{\pi}}$, and comparison is made with the phenomenological expressions for these quantities, H-5 and H-9 are obtained for the thermal conductivity and shear viscosity tensors, respectively:

$$\underline{\underline{\lambda}} = \left(\frac{2k_B}{mT}\right)^{1/2} n\langle\langle(k_B T W^2 + H_{int})\underline{W}|\underline{A}\rangle\rangle \qquad (I.1-3)$$

and

$$\underline{\underline{p}} = nk_BT \langle\langle [\underline{W}]^{(2)} | \underline{\underline{B}} \rangle\rangle . \qquad (I.1-4)$$

In the above, k_B is the Boltzmann constant, m is the mass of a gas molecule, $\underline{W} = (2mk_BT)^{-1/2}\, \underline{p}$ is the reduced peculiar velocity, H_{int} is the internal Hamiltonian of a single molecule, and the inner product is defined as in H-6:

$$\langle\langle \underline{\underline{a}} | \underline{\underline{b}} \rangle\rangle = n^{-1}\, Tr \int d\underline{p}\; f^{(0)}\, \underline{\underline{a}}^{+}\, \underline{\underline{b}} , \qquad (I.1-5)$$

in which $^{+}$ denotes the adjoint operator, and the trace is over internal states.

Due to the independence of macroscopic gradients, the linearized Waldmann-Snider equation becomes separate equations[6] for $\underline{A}$ and $\underline{\underline{B}}$:

$$(\mathcal{R} + iL)\underline{A} = \left(\frac{2k_BT}{m}\right)^{1/2} \left\{ W^2 - \frac{5}{2} + \left[\frac{H_{int} - \langle H_{int}\rangle}{k_BT}\right] \right\} \underline{W} \qquad (I.1-6)$$

and

$$(\mathcal{R} + iL)\underline{\underline{B}} = 2[\underline{W}]^{(2)} , \qquad (I.1-7)$$

in which $\langle H_{int}\rangle \equiv \langle\langle H_{int} | 1 \rangle\rangle$, $\mathcal{R}$ is the linearized Waldmann-Snider collision superoperator, and L is the Larmor precession superoperator defined by H-13.

$$\mathcal{L}\Phi = \omega_L [J_Z, \Phi] \ . \qquad (I.1\text{-}8)$$

In the above, J_Z is the component of internal angular momentum operator along the field, and ω_L is the Larmor frequency:

$$\omega_L = \frac{g\mu_N}{\hbar} H_M \ , \qquad (I.1\text{-}9)$$

where g is the rotational Landé g-factor, μ_N the nuclear magneton, and H_M the magnetic field strength.

Using the tensor equations just obtained, along with the auxiliary condition of H-14,

$$\langle\langle \underline{W} | \underline{A} \rangle\rangle = 0 \ , \qquad (I.1\text{-}10)$$

scalar equations are obtained for $\underline{\underline{\lambda}}$ and $\underline{\underline{\eta}}$ by considering two bases, the projection operator basis,[4,5]

$$\underline{\underline{A}}_{pqsj} \equiv \underline{\underline{L}}^{ps}(\underline{W})\ \mathcal{Y}^{(q)}(\underline{J})\ P_j (p_j)^{-1/2} , \qquad (I.1\text{-}11)$$

in which $\underline{\underline{L}}^{ps}(\underline{W})$ is a p-th rank tensor-valued function of $\underline{W}$, $\mathcal{Y}^{(q)}(\underline{J})$ is a q-th rank tensor operator dependent on the internal angular momentum operator, $\underline{J}$, of one molecule, P_j is a projection operator onto the j-th energy level, and p_j is the Boltzmann weight of the j-th level; and the Wang Chang-Uhlenbeck basis,[4]

$$\underline{\underline{B}}_{pqst} = \underline{\underline{L}}^{ps}(\underline{W})[\underline{\underline{J}}]^{(q)} R_t^{(q)}\left(\frac{H_{int}}{k_B T}\right) , \tag{I.1-12}$$

in which $R_t^{(q)}$ is a normalized Wang Chang-Uhlenbeck polynomial and $[\underline{\underline{J}}]^{(q)}$ is a q-th rank symmetric traceless tensor of $\underline{J}$, e.g. $[\underline{\underline{J}}]^{(2)} = \underline{J}\underline{J} - \frac{1}{3}J^2\underline{\underline{U}}$, where $\underline{\underline{U}}$ is the second rank unit tensor. The matrix elements of R and L in these two bases are given in H-24, H-25, H-40, and H-41:

$$\langle\langle A^{(a)\alpha}_{pqsj}|R|A^{(a')\alpha'}_{p'q's'j'}\rangle\rangle$$
$$= n\left(\frac{m}{8k_B T}\right)^{-1/2} (2a+1)^{-1} \sigma(pqsj|p'q's'j')^{(a)} \delta_{a\alpha,a'\alpha'} , \tag{I.1-13}$$

$$\langle\langle A^{(a)\alpha}_{pqsj}|L|A^{(a')\alpha'}_{p'q's'j'}\rangle\rangle = L^{(\alpha)}_{pq}(aa') \delta_{pqsj,p'q's'j'} \delta_{\alpha,\alpha'} , \tag{I.1-14}$$

$$\langle\langle B^{(a)\alpha}_{pqst}|R|B^{(a')\alpha'}_{p'q's't'}\rangle\rangle = n\left(\frac{m}{8k_B T}\right)^{-1/2} (2a+1)^{-1} \begin{pmatrix} p\ q\ s\ t \\ p'q's't' \end{pmatrix}^{(a)} \delta_{a\alpha,a'\alpha'} , \tag{I.1-15}$$

and

$$\langle\langle B^{(a)\alpha}_{pqst}|L|B^{(a')\alpha'}_{p'q's't'}\rangle\rangle = L^{(\alpha)}_{pq}(aa') \delta_{pqst,p'q's't'} \delta_{\alpha,\alpha'} . \tag{I.1-16}$$

In the above, m is the reduced mass of the collision pair, and $A^{(a)\alpha}_{pqsj}$ and $B^{(a)\alpha}_{pqst}$ are spherical components of the total

polarization bases of $\underline{A}_{pqsj}$ and $\underline{B}_{pqst}$, respectively. Expressions for $L_{pq}^{(\ell)}(aa')$ are given in Ref. 1.

The spherical components of $\underline{A}$ and $\underline{\underline{B}}$ are then expanded over the total polarization basis, $B_{pqst}^{(a)\alpha}$, to obtain

$$A^m = \sum_{pqsta} (1 - \delta_{pqst,1000})\, A_{(a)m}^{pqst}\, B_{pqst}^{(a)m} \qquad (I.1\text{-}17)$$

(the $1-\delta_{pqst,1000}$ factor ensuring that the auxiliary condition expressed in equation (I.1-10) is satisfied) and

$$B^m = \sum_{pqsta} B_{(a)m}^{pqst}\, B_{pqst}^{(a)m}, \qquad (I.1\text{-}18)$$

where $A_{(a)m}^{pqst}$ and $B_{(a)m}^{pqst}$ are expansion coefficients given by the following matrix equations:

$$n\left(\frac{\pi\mu}{8k_B T}\right)^{-1/2} (2a+1)^{-1} \sum_{p'q's't'} \sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)} A_{(a)m}^{p'q's't'}$$

$$+\, i(1-\delta_{pqst,1000}) \sum_{a'} L_{pq}^{(m)}(aa') A_{(a')m}^{pqst}$$

$$= \left(\frac{c_{int}T}{3m}\right)^{1/2} \delta_{a,1}\left[\delta_{pqst,1001} - \left(\frac{5k_B}{2c_{int}}\right)^{1/2} \delta_{pqst,1010}\right] \qquad (I.1\text{-}19)$$

and

$$\sum_{p'q's't'a'} \left\{ \delta_{a,a'}\, n \left(\frac{\pi\mu}{8k_B T}\right)^{-1/2} (2a+1)^{-1}\, \sigma \begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)} \right.$$

$$\left. + i\delta_{pqst,p'q's't'}\, L^{(m)}_{pq}(aa') \right\} B^{p'q's't'}_{(a')m}$$

$$= \left(\frac{2}{5}\right)^{1/2} \delta_{pqst,2000}\, \delta_{a,2}\ , \qquad \text{(I.1-20)}$$

in which c_{int} is the internal heat capacity per molecule. The spherical components of $\underline{\underline{\lambda}}$ and $\underline{\underline{\eta}}$ are then given by

$$\lambda_m = nk_B \left(\frac{c_{int}T}{3m}\right)^{1/2} \left[A^{1001}_{(1)m} - \left(\frac{5k_B}{2c_{int}}\right)^{1/2} A^{1010}_{(1)m}\right] \qquad \text{(I.1-21)}$$

and

$$\eta_m = \frac{1}{\sqrt{10}}\, nk_B T\, B^{2000}_{(2)m}\ . \qquad \text{(I.1-22)}$$

The important point of Hunter's development of the transport coefficients is that the tensor analysis precedes any truncation of the basis. Solutions to (I.1-19) and (I.1-20) require the truncation of the basis and evaluation of the scalars, $\sigma \begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$. The remainder of Part I is concerned with the evaluation of these scalars. With the ultimate goal of obtaining calculated values of these scalars, they are expressed in terms of relative momentum collision integrals in section I.2, which in turn are written in terms of the reduced scattering matrix of Curtiss and co-workers[7] in sections I.3 and I.5 and simplified by the introduction of various operators in sections I.4 and I.6.

Finally, some interesting relations among the scalars, suggested by similar relations found by Chen, Moraal, and Snider[4] for the collision integrals in another representation, are developed in section I.7.

I.2 Expansion of the $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$ in Terms of the Relative Momentum Collision Integrals

The $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$ provide a description of the collision process in terms of initial and final momenta (psp's') of a single molecule. In order to express these quantities in terms of $S(j_a'j_b'\lambda|S_aS_b)$, the reduced scattering matrix, it is first necessary to make the transition to a description of the collision process in terms of initial and final relative momenta ($\kappa n \kappa' n'$) of the collision pair. This is accomplished through the introduction of the quantity[4] $I^{(k)}_{\kappa n \kappa' n';psp's'}$, defined in CMS-B16 and resulting from the transformation to center of mass and relative coordinates. This section is concerned with obtaining expressions for the $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$ in terms of the $\sigma'\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k$ and $\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k$ relative momentum collision integrals.

The scalars $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$ defined in H-40 and (I.1-15) are related[1] to the scalars $\sigma(pqsj_a|p'q's'j_a')^{(a)}$ defined in H-24 and (I.1-13):

$$\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)} = \sum_{j_a j_a'} \alpha^{-1}(qq')(p_{j_a j_a'})^{1/2} \left([\underline{J}]^{(q)} \odot^q [\underline{J}]^{(q)}\right)^{1/2}_{j_a}$$

$$\times\left([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')}\right)^{1/2}_{j_a'} R_t^{(q)}(\varepsilon_{j_a}) R_{t'}^{(q')}(\varepsilon_{j_a'})\, \sigma(pqsj_a|p'q's'j_a')^{(a)} \qquad \text{(I.2-1)}$$

in which $\alpha(\ell_1\ell_2\cdots) = \sqrt{(2\ell_1+1)(2\ell_2+1)\cdots}$,

$\varepsilon_{j_a} = (E_{j_a}/k_BT) = (\hbar^2 j_a(j_a+1))/(2I_ak_BT)$ is the dimensionless

rotational energy of molecule a, and
$(p_{j_a j_a'})^{1/2} \equiv (p_{j_a})^{1/2}(p_{j_a'})^{1/2} = \alpha(j_a j_a')Q^{-1}\exp(-\varepsilon_{j_a}-\varepsilon_{j_a'})$, Q being the molecular partition function. The quantity $([\underline{\underline{J}}]^{(q)}\odot\mathcal{A}[\underline{\underline{J}}]^{(q)})^{1/2}_{j_a}$ is introduced in Ref. 4.

Using H-27 and HS-19, the scalars $\sigma(pqsj_a|p'q's'j_a')^{(a)}$ can be expressed in terms of the scalars $\sigma(pqsj_a|p'q's'j_a')_k$, which in turn can be expressed in terms of the cross sections, $\sigma'(\ell n j_a j_b q|\ell' n' j_a' j_b' q')_k$ *and* $\sigma''(\ell n j_a j_b q|\ell' n' j_b' j_a' q')_k$. Substitution of these expressions in (I.2-1) yields

$$\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}$$

$$= (-1)^{q+a+p'}\sum_k (-1)^k \alpha^2(k)\Omega(kq'q)^{1/2}\Omega(kp'p)^{1/2}\Omega(kpp')^{-1/2}\begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}$$

$$\times \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2}\, I^{(k)}_{\ell n \ell' n'; psp's'} \sum_{\substack{j_a j_b \\ j_a' j_b'}} (p_{j_a j_b j_a' j_b'})^{1/2}$$

$$\times ([\underline{\underline{J}}]^{(q)}\odot\mathcal{A}[\underline{\underline{J}}]^{(q)})^{1/2}_{j_a}\,([\underline{\underline{J}}]^{(q')}\odot\mathcal{A}'[\underline{\underline{J}}]^{(q')})^{1/2}_{j_a'}$$

$$\times R_t^{(q)}(\varepsilon_{j_a})\,R_{t'}^{(q')}(\varepsilon_{j_a'})\,\alpha^{-1}(qq')$$

$$\times \left\{\sigma'(\ell n j_a j_b q|\ell' n' j_a' j_b' q')_k + (-1)^{\ell'}\sigma''(\ell n j_a j_b q|\ell' n' j_b' j_a' q')_k\right\}. \tag{I.2-2}$$

The quantities $\Omega(\ell_1\ell_2\ell_3)$ are defined in CMS-A22 and $\begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}$ is a 6-j symbol.[8]

H-63 defines a new scalar which can be written

$$\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}_k$$

$$= \alpha^2(k)\Omega(kp'p)^{-1/2} \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2}\, I^{(k)}_{\ell n \ell' n';psp's'}$$

$$\times \sum_{\substack{j_a j_b \\ j'_a j'_b}} (p_{j_a j_b j'_a j'_b})^{1/2} ([\underline{J}]^{(q)} \odot^q [\underline{J}]^{(q)})^{1/2}_{j_a} ([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')})^{1/2}_{j'_a}$$

$$\times R^{(q)}_t(\varepsilon_{j_a})\, R^{(q')}_{t'}(\varepsilon_{j'_a})\, \alpha^{-1}(qq')$$

$$\times \left\{\sigma'(\ell n j_a j_b q|\ell' n' j'_a j'_b q')_k + (-1)^{\ell'}\, \sigma''(\ell n j_a j_b q|\ell' n' j'_b j'_a q')_k\right\} . \tag{I.2-3}$$

This can be rewritten as

$$\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}_k = \alpha^2(k)\Omega(kp'p)^{-1/2} \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2}\, I^{(k)}_{\ell n \ell' n';psp's'}$$

$$\times \left\{\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k + (-1)^{\ell'}\, \sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k\right\} \tag{I.2-4}$$

if two new collision integrals are defined:

$$\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k \equiv \sum_{\substack{j_a j_b \\ j'_a j'_b}} (p_{j_a j_b j'_a j'_b})^{1/2}$$

$$\times ([\underline{\underline{J}}]^{(q)} \mathcal{A} [\underline{\underline{J}}])^{(q)})^{1/2}_{j_a} ([\underline{\underline{J}}]^{(q')} \mathcal{A}' [\underline{\underline{J}}]^{(q')})^{1/2}_{j'_a}$$

$$\times \alpha^{-1}(qq') R_t^{(q)}(\varepsilon_{j_a}) R_{t'}^{(q')}(\varepsilon_{j'_a}) \; \sigma'(\ell n j_a j_b q | \ell' n' j'_a j'_b q')_k \quad \text{(I.2-5)}$$

and

$$\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k \equiv \sum_{\substack{j_a j_b \\ j'_a j'_b}} (p_{j_a j_b j'_a j'_b})^{1/2}$$

$$\times ([\underline{\underline{J}}]^{(q)} \mathcal{A} [\underline{\underline{J}}]^{(q)})^{1/2}_{j_a} ([\underline{\underline{J}}]^{(q')} \mathcal{A}' [\underline{\underline{J}}]^{(q')})^{1/2}_{j'_a}$$

$$\times \alpha^{-1}(qq') R_t^{(q)}(\varepsilon_{j_a}) R_{t'}^{(q')}(\varepsilon_{j'_a}) \; \sigma''(\ell n j_a j_b q | \ell' n' j'_b j'_a q')_k . \quad \text{(I.2-6)}$$

These are the desired relative momentum collision integrals. The $\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}$ scalars can now be written

$$\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)} = \sum_k \Omega(kq'q)^{1/2} \; \Omega(kp'p)^{1/2} \; (-1)^{k+q+a+p'}$$

$$\times \begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix} \sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}_k$$

$$= (-1)^{q+a+p'} \sum_k (-1)^k \; \alpha^2(k) \; \Omega(kq'q)^{1/2} \begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}$$

$$\times \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2} \; I^{(k)}_{\ell n \ell' n'; psp's'}$$

$$\times \left\{ \sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k + (-1)^{\ell'} \; \sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k \right\} . \quad \text{(I.2-7)}$$

After lengthy substitutions, the $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ relative momentum collision integrals can be expressed in terms of the reduced scattering matrix, $S(j_a'j_b'\lambda|S_aS_b)$, and consequently, in terms of the generalized phase shift, $H(j_a'j_b'\lambda|S_aS_b)$, of Curtiss and co-workers.[7] Considerable algebraic manipulation and the introduction of various operators allows the expressions for $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ to be greatly simplified. These substitutions and simplifications are carried out in the next four sections.

I.3 $\sigma'\begin{Bmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{Bmatrix}_k$ *in Terms of the Reduced Scattering Matrix*

Equation (I.2-5) is an expression for $\sigma'\begin{Bmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{Bmatrix}_k$ in terms of the kinetic theory cross section, $\sigma'(\ell n j_a j_b q|\ell' n' j_a' j_b' q')_k$, for nonvibrating diatomic molecules. HS-43 gives an expression for $\sigma'(\ell n j_a j_b q|\ell' n' j_a' j_b' q')_k$ in terms of the relative velocity cross sections, $\sigma_1(\ell n|j_a j_b;k0|\ell' n')_k$ and $\sigma_2(\ell n j_a j_b|L_a M_a L_b M_b;L_a' M_a' L_b M_b|\ell' n' j_a' j_b')_k$. Substitution of this expression in (I.2-5) yields

$$
\begin{aligned}
\sigma'\begin{Bmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{Bmatrix}_k = {} & \Omega(kqq')^{-1/2}\, i^{q+q'} \Bigg\{\Bigg[\sum_{j_a' j_b'} (-1)^k \alpha^{-1}(k)\alpha(j_a')(p_{j_a' j_b'}) \\
& \times \left([\underline{J}]^{(q)} \odot^{q} [\underline{J}]^{(q)}\right)^{1/2}_{j_a'} \left([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')}\right)^{1/2}_{j_a'} R_t^{(q)}(\varepsilon_{j_a'}) R_{t'}^{(q')}(\varepsilon_{j_a'}) \\
& \times \begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & k \end{Bmatrix} \left[\sigma_1(\ell n|j_a' j_b';k0|\ell' n')_k + (-1)^{q+q'} \sigma(\ell n|j_a' j_b';k0|\ell' n')_k^*\right]\Bigg] \\
& - \Bigg[\sum_{\substack{j_a j_b \\ j_a' j_b'}} (-1)^q \alpha^{-1}(j_b)\alpha^2(j_a')\alpha(j_b')(p_{j_a j_b j_a' j_b'})^{1/2} \\
& \times \left([\underline{J}]^{(q)} \odot^{q} [\underline{J}]^{(q)}\right)^{1/2}_{j_a} \left([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')}\right)^{1/2}_{j_a'} R_t^{(q)}(\varepsilon_{j_a}) R_{t'}^{(q')}(\varepsilon_{j_a'}) \\
& \times \sum_{\substack{L_a L_a' L_b \\ M_a M_a' M_b}} \begin{Bmatrix} q' & q & k \\ j_a' & j_a & L_a \\ j_a' & j_a & L_a' \end{Bmatrix} \alpha(L_a L_a')(-1)^{L_a'+M_b} \begin{pmatrix} L_a & L_a' & k \\ M_a & -M_a' & M_a'-M_a \end{pmatrix} \\
& \times \sigma_2(\ell n j_a j_b|L_a M_a L_b M_b;L_a' M_a' L_b M_b|\ell' n' j_a' j_b')_k\Bigg]\Bigg\}, \qquad \text{(I.3-1)}
\end{aligned}
$$

in which $\begin{Bmatrix} q' & q & k \\ j_a' & j_a & L_a \\ j_a' & j_a & L_a' \end{Bmatrix}$ is a 9-j symbol.[8]

The relative velocity cross sections are expressed in terms of quantities $F_\lambda(j_a'j_b';L_aM_aL_bM_b;j_aj_b)$ with the aid of HS-41 and HS-42:

$$\sigma_1(\ell n|j_a'j_b';k0|\ell'n')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2} \Omega(k\ell\ell')^{-1/2}(-i)^{\ell+\ell'}(-1)^k\alpha(\ell\ell')$$
$$\times \begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} \int d\gamma \frac{\gamma^2}{\mu g} R_{n\ell}(\gamma)R_{n'\ell'}(\gamma) \sum_\lambda \alpha^2(\lambda)\, F_\lambda(j_a'j_b';k000;j_a'j_b') \quad \text{(I.3-2)}$$

and

$$\sigma_2(\ell n j_a j_b|L_aM_aL_bM_b;L_a'M_a'L_bM_b|\ell'n'j_a'j_b')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2}\Omega(k\ell\ell')^{-1/2}(-i)^{\ell+\ell'}\alpha(\ell\ell')$$
$$\times \begin{pmatrix} k & \ell & \ell' \\ M_a-M_a' & 0 & M_a'-M_a \end{pmatrix} \int d\gamma\gamma^2 \int dg'(g')^2 \frac{\delta(E)}{gg'} R_{n\ell}(\gamma)R_{n'\ell'}(\gamma')$$
$$\times \sum_{\lambda\lambda'} \alpha^2(\lambda\lambda') \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & -M_a'-M_b & M_a'-M_a \end{pmatrix}$$
$$\times F_\lambda(j_a'j_b';L_aM_aL_bM_b;j_aj_b)\, F^*_{\lambda'}(j_a'j_b';L_a'M_a'L_bM_b;j_aj_b)\,. \quad \text{(I.3-3)}$$

In the above, g' and g are the relative velocities of the centers of mass of the colliding molecules before and after collision, while γ' and γ are the dimensionless relative velocities (momenta) before and after collision. The $R_{n\ell}(\gamma)$ are normalized three-dimensional harmonic oscillator wavefunctions introduced in CMS-74.

The F_λ quantitie ·:pearing in the relative velocity cross sections are normalizeu ıch that for a spherical interaction potential, $V = V^{(0)}$,

$$F_\lambda(j_a'j_b';L_aM_aL_bM_b;j_aj_b)_{\text{spherical}} = \delta(L_aM_aL_bM_b|0000)\ \delta(j_a'j_b'|j_aj_b) \times [1 - \exp(2i\eta_\lambda)] , \qquad \text{(I.3-4)}$$

η_λ being the spherical phase shift. Thus, the F_λ are a type of reduced transition matrix. In terms of $S(j_a'j_b'\lambda|S_aS_b)$, the reduced scattering matrix,[5]

$$\begin{aligned} F_\lambda(j_a'j_b';L_aM_aL_bM_b;j_aj_b) &= (-1)^{j_a'+j_b'}(-i)^{M_a+M_b}\,\alpha(j_aj_b)\,\alpha(L_aL_b) \\ &\times (8\pi^2)^{-2}\sum_{\nu\mu}(-i)^{\nu+\mu}\begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu\end{pmatrix}\begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu\end{pmatrix} \\ &\times \iint dS_a\,dS_b\,[1 - S(j_a'j_b'\lambda|S_aS_b)]D^{L_a}_{\nu M_a}(S_a)\,D^{L_b}_{\mu M_b}(S_b) , \qquad \text{(I.3-5)}\end{aligned}$$

where $\begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu\end{pmatrix}$ is a 3-j symbol and the $D^{L_a}_{\nu M_a}(S_a)$ are elements of the rotation matrix.[8]

Insertion of equation (I.3-5) in equations (I.3-2) and (I.3-3) leads to expressions for the relative velocity cross sections in terms of the reduced scattering matrix:

$$\sigma_1(\ell n|j_a'j_b';k0|\ell'n')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2} \sum_\lambda \alpha^2(\lambda)$$

$$\times\Big\{[\Omega(0\ell\ell)^{-1/2}\ \alpha(\ell)\ \delta(\ell k|\ell'0) \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma)R_{n'\ell}(\gamma)]$$

$$-\ [\Omega(k\ell\ell')^{-1/2}\ (-i)^{\ell+\ell'}\ (-1)^{k+j_a'}\ \alpha(j_a'k)\alpha(\ell\ell')\begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0\end{pmatrix}$$

$$\times \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma)R_{n'\ell'}(\gamma) \sum_\nu (-i)^\nu \begin{pmatrix} j_a' & j_a' & k \\ 0 & \nu & -\nu\end{pmatrix} (8\pi^2)^{-2}$$

$$\times \iint dS_a\ dS_b\ S(j_a'j_b'\lambda|S_aS_b)\ D^k_{\nu 0}(S_a)]\Big\} \qquad \text{(I.3-6)}$$

and

$$\sigma_2(\ell nj_aj_b|L_aM_aL_bM_b;L_a'M_a'L_bM_b|\ell'n'j_a'j_b')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2}$$

$$\times\Big\{\Big[\Omega(k\ell\ell)^{-1/2}\ (-1)^\ell\ \alpha^2(\ell)\begin{pmatrix} k & \ell & \ell \\ 0 & 0 & 0\end{pmatrix}$$

$$\times\ \delta(\ell|\ell')\delta(j_aj_b|j_a'j_b')\delta(L_aL_a'L_b|000)\delta(M_aM_a'M_b|000)$$

$$\times \sum_\lambda \alpha^2(\lambda) \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma)\ R_{n'\ell}(\gamma)\Big]$$

$$-\ \Big[\Omega(k\ell\ell')^{-1/2}\ (-i)^{\ell+\ell'}\ (-1)^{j_a'}\ \alpha(\ell\ell')\alpha(j_a')\ \delta(j_aj_b|j_a'j_b')\delta(L_bM_b|00)$$

$$\times \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma)\ R_{n'\ell'}(\gamma) \sum_{\lambda\lambda'\nu} \alpha^2(\lambda\lambda')\begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0\end{pmatrix}(8\pi^2)^{-2} \iint dS_a\ dS_b$$

$$\times \Big[\delta(L_a'M_a'|00)(-i)^{M_a+\nu}\ \alpha(L_a)\begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a & 0 & -M_a\end{pmatrix}\begin{pmatrix} k & \ell & \ell' \\ M_a & 0 & -M_a\end{pmatrix}\begin{pmatrix} j_a' & j_a' & L_a \\ 0 & \nu & -\nu\end{pmatrix}$$

$$\times\ S\ (j_a'j_b'\lambda|S_aS_b)\ D^{L_a}_{\nu M_a}(S_a)\ \Big]\Big] + \delta(L_aM_a|00)(-i)^{-M_a'-\nu}\ \alpha(L_a') \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a' & 0 & -M_a'\end{pmatrix}$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ M_a' & 0 & -M_a'\end{pmatrix}\begin{pmatrix} j_a' & j_a' & L_a' \\ 0 & \nu & -\nu\end{pmatrix}\ S^*(j_a'j_b'\lambda|S_aS_b)D^{L_a'}_{\nu M_a'}(S_a)^*$$

(Equation continued on following page.)

$$+\left[\Omega(k\ell\ell')^{-1/2}(-i)^{\ell+\ell'}\alpha(\ell\ell')\int d\gamma\,\gamma^2\int dg'(g')^2\,\frac{\delta(E)}{gg'}\,R_{n\ell}(\gamma)R_{n'\ell'}(\gamma')\right.$$

$$\times\sum_{\lambda\lambda'}\alpha^2(\lambda\lambda')\begin{pmatrix}\lambda&\lambda'&\ell'\\0&0&0\end{pmatrix}\begin{pmatrix}\lambda&\lambda'&\ell'\\M_a+M_b&-M_a'-M_b&M_a'-M_a\end{pmatrix}\begin{pmatrix}k&\ell&\ell'\\M_a-M_a'&0&M_a'-M_a\end{pmatrix}$$

$$\times(-i)^{M_a-M_a'}\alpha^2(j_aj_b)\alpha^2(L_b)\alpha(L_aL_a')\sum_{\substack{\nu\mu\\\nu'\mu'}}(-i)^{\nu+\mu-\nu'-\mu'}$$

$$\times\begin{pmatrix}j_a&j_a'&L_a\\0&\nu&-\nu\end{pmatrix}\begin{pmatrix}j_b&j_b'&L_b\\0&\mu&-\mu\end{pmatrix}\begin{pmatrix}j_a&j_a'&L_a'\\0&\nu'&-\nu'\end{pmatrix}\begin{pmatrix}j_b&j_b'&L_b\\0&\mu'&-\mu'\end{pmatrix}$$

$$\times(8\pi^2)^{-4}\iiiint dS_a\,dS_b\,dS_a'\,dS_b'\;\mathcal{S}(j_a'j_b'\lambda|S_aS_b)\;\mathcal{S}^*(j_a'j_b'\lambda'|S_a'S_b')$$

$$\left.\left.\times D^{L_a}_{\nu M_a}(S_a)\;D^{L_b}_{\mu M_b}(S_b)\;D^{L_a'}_{\nu' M_a'}(S_a')^*\;D^{L_b}_{\mu' M_b}(S_b')^*\right]\right\}. \qquad \text{(I.3-7)}$$

At this stage it is useful to consider the terms of $\sigma'\begin{pmatrix}\ell&q&n&t\\\ell'&q'&n'&t'\end{pmatrix}_k$ involving relative velocity cross sections as they appear in equation (I.3-1):

$$\Omega(kqq')^{-1/2}\,(i)^{q+q'}\sum_{j_a'j_b'}(-1)^k\,\alpha^{-1}(k)\alpha(j_a')(p_{j_a'j_b'})\left([\underline{J}]^{(q)}\odot^q[\underline{J}]^{(q)}\right)^{1/2}_{j_a'}$$

$$\times\left([\underline{J}]^{(q')}\odot^{q'}[\underline{J}]^{(q')}\right)^{1/2}_{j_a'}\,R_t^{(q)}(\varepsilon_{j_a'})R_{t'}^{(q')}(\varepsilon_{j_a'})$$

$$\times\begin{Bmatrix}j_a'&q&j_a'\\q'&j_a'&k\end{Bmatrix}\sigma_1(\ell n|j_a'j_b';k0|\ell'n')_k$$

$$=\frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2}\sum_{j_a'j_b'}\sum_{\lambda}\alpha^2(\lambda)\left\{\left[\Omega(0qq)^{-1/2}\Omega(0\ell\ell)^{-1/2}\alpha^{-1}(q)\alpha(\ell)\delta(\ell qk|\ell'q'0)\right.\right.$$

(Equation continued on next page.)

$$\times\ (p_{j_a' j_b'})([\underline{J}]^{(q)} \odot^q [\underline{J}]^{(q)})_{j_a'} R_t^{(q)}(\varepsilon_{j_a'}) R_{t'}^{(q)}(\varepsilon_{j_a'}) \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma) R_{n'\ell}(\gamma)\Big]$$

$$-\ \Big[\Omega(kqq')^{-1/2}\Omega(k\ell\ell')^{-1/2}(i)^{q+q'-\ell-\ell'}\ (-1)^{j_a'}\ \alpha^2(j_a')\ \alpha(\ell\ell')(p_{j_a' j_b'})$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & k \end{Bmatrix} ([\underline{J}]^{(q)} \odot^q [\underline{J}]^{(q)})^{1/2}_{j_a'} ([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')})^{1/2}_{j_a'}$$

$$\times\ R_t^{(q)}(\varepsilon_{j_a'}) R_{t'}^{(q')}(\varepsilon_{j_a'})\ \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma)\ R_{n'\ell'}(\gamma)$$

$$\times \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a' & j_a' & k \\ 0 & \nu & -\nu \end{pmatrix} (8\pi^2)^{-2} \iint dS_a dS_b\ S(j_a' j_b' \lambda | S_a S_b) D^k_{\nu 0}(S_a)\Big]\Big\}\ , \tag{I.3-8}$$

since[8,9] $\begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & 0 \end{Bmatrix} = (-1)^q\ \alpha^{-1}(j_a' q)\ \delta(q|q')$. The j_a' and j_b' summations appearing in the first term above can be carried out:[4]

$$\sum_{j_a' j_b'} (p_{j_a' j_b'})([\underline{J}]^{(q)} \odot^q [\underline{J}]^{(q)})_{j_a'}\ R_t^{(q)}(\varepsilon_{j_a'}) R_{t'}^{(q)}(\varepsilon_{j_a'})\ =\ \alpha^2(q)\ \delta_{tt'}\ , \tag{I.3-9}$$

allowing the right side of equation (I.3-8) to be written as

$$=\ \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_B T}\right)^{1/2}\ \sum_{\lambda} \alpha^2(\lambda)\Big\{\big[\Omega(0qq)^{-1/2}\Omega(0\ell\ell)^{-1/2}\ \alpha(\ell q)\ c(\ell q t k|\ell' q' t' 0)$$

$$\times \int d\gamma\ \frac{\gamma^2}{\mu g}\ R_{n\ell}(\gamma)\ R_{n'\ell}(\gamma)\big]$$

$$-\ \sum_{j_a' j_b'} [\Omega(kqq')^{-1/2}\ \Omega(k\ell\ell')^{-1/2}\ (i)^{q+q'-\ell-\ell'}(-1)^{j_a'}\ \alpha^2(j_a')\ \alpha(\ell\ell')$$

(Equation continued on following page.)

$$\times\ (p_{j_a' j_b'}) \begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & k \end{Bmatrix} \left([\underline{J}]^{(q)} \odot \mathcal{A} [\underline{J}]^{(q)}\right)^{1/2}_{j_a'} \left([\underline{J}]^{(q')} \odot \mathcal{A}' [\underline{J}]^{(q')}\right)^{1/2}_{j_a'}$$

$$\times\ R_t^{(q)}(\varepsilon_{j_a'}) R_{t'}^{(q')}(\varepsilon_{j_a'}) \int d\gamma\, \frac{\gamma^2}{\mu g}\, R_{n\ell}(\gamma)\, R_{n'\ell'}(\gamma)$$

$$\times \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a' & j_a' & k \\ 0 & \nu & -\nu \end{pmatrix} (8\pi^2)^{-2} \iint dS_a dS_b\, S(j_a' j_b' \lambda | S_a S_b) D^{k}_{\nu 0}(S_a)]\Big\} . \qquad (I.3\text{-}10)$$

The above expression involves a constant term and a term linear in the reduced scattering matrix, a result of the fact that the σ_1 cross section is linear in the transtion matrix.[5]

The σ_2 cross section, on the other hand, is bilinear in the transition matrix,[5] and consequently, this term is somewhat more difficult to evaluate:

$$\Omega(kqq')^{-1/2}(i)^{q+q'}(-1)^q \sum_{\substack{j_a j_b \\ j_a' j_b'}} \alpha^{-1}(j_b)\alpha^2(j_a')\alpha(j_b')(p_{j_a j_b j_a' j_b'})^{1/2}$$

$$\times \left([\underline{J}]^{(q)} \odot \mathcal{A} [\underline{J}]^{(q)}\right)^{1/2}_{j_a} \left([\underline{J}]^{(q')} \odot \mathcal{A}' [\underline{J}]^{(q')}\right)^{1/2}_{j_a'} R_t^{(q)}(\varepsilon_{j_a}) R_{t'}^{(q')}(\varepsilon_{j_a'})$$

$$\times \sum_{\substack{L_a L_a' L_b \\ M_a M_a' M_b}} \begin{Bmatrix} q' & q & k \\ j_a' & j_a & L_a \\ j_a' & j_a & L_a' \end{Bmatrix} \alpha(L_a L_a')(-1)^{L_a' + M_b} \begin{pmatrix} L_a & L_a' & k \\ M_a & -M_a' & M_a' - M_a \end{pmatrix}$$

$$\times\ \sigma_2(\ell n j_a j_b | L_a M_a L_b M_b ; L_a' M_a' L_b M_b | \ell' n' j_a' j_b')_k$$

(Equation continued on following page.)

$$= \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2} \Omega(kqq')^{-1/2}\, (i)^{q+q'}\, (-1)^q \sum_{\substack{j_aj_b\\ j_a'j_b'}} \alpha^{-1}(j_b)\alpha^2(j_a')\alpha(j_b')$$

$$\times\, (p_{j_aj_bj_a'j_b'})^{1/2}\, \left([\underline{J}]^{(q)}\odot\mathcal{A}[\underline{J}]^{(q)}\right)_{j_a}^{1/2}\, \left([\underline{J}]^{(q')}\odot\mathcal{A}'[\underline{J}]^{(q')}\right)_{j_a'}^{1/2}$$

$$\times\, R_t^{(q)}(\varepsilon_{j_a})R_{t'}^{(q')}(\varepsilon_{j_a'})\, \Big\{[\Omega(k\ell\ell)^{-1/2}\, (-1)^{\ell}\, \alpha^2(\ell)\, \delta_{\ell\ell'} \begin{pmatrix} k & \ell & \ell \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{Bmatrix} q' & q & k \\ j_a' & j_a' & 0 \\ j_a' & j_a' & 0 \end{Bmatrix} \begin{pmatrix} 0 & 0 & k \\ 0 & 0 & 0 \end{pmatrix} \delta(j_aj_b|j_a'j_b') \sum_{\lambda} \alpha^2(\lambda) \int d\gamma\, \frac{\gamma^2}{\mu g}\, R_{n\ell}(\gamma)R_{n'\ell}(\gamma)]$$

$$- \Omega(k\ell\ell')^{-1/2}\, (-i)^{\ell+\ell'}\, \alpha(\ell\ell')(-1)^{j_a'}\, \alpha(j_a')\, \delta(j_aj_b|j_a'j_b')$$

$$\times \int d\gamma\, \frac{\gamma^2}{\mu g}\, R_{n\ell}(\gamma)R_{n'\ell'}(\gamma) \sum_{\lambda\lambda'\nu} \alpha^2(\lambda\lambda') \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} (8\pi^2)^{-2} \iint dS_a\, dS_b$$

$$\times \Bigg[\Bigg(\sum_{L_aM_a} \begin{Bmatrix} q' & q & k \\ j_a' & j_a' & L_a \\ j_a' & j_a' & 0 \end{Bmatrix} \alpha^2(L_a) \begin{pmatrix} L_a & 0 & k \\ M_a & 0 & -M_a \end{pmatrix} (-i)^{M_a+\nu}$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ M_a & 0 & -M_a \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a & 0 & -M_a \end{pmatrix} \begin{pmatrix} j_a' & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} S(j_a'j_b'\lambda|S_aS_b) D^{L_a}_{\nu M_a}(S_a)\Bigg)$$

$$+ \Bigg(\sum_{L_a'M_a'} \begin{Bmatrix} q' & q & k \\ j_a' & j_a' & 0 \\ j_a' & j_a' & L_a' \end{Bmatrix} \alpha^2(L_a')(-1)^{L_a'} \begin{pmatrix} 0 & L_a' & k \\ 0 & -M_a' & M_a' \end{pmatrix} (-i)^{-M_a'-\nu}$$

$$\times \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a' & 0 & -M_a' \end{pmatrix} \begin{pmatrix} k & \ell & \ell' \\ M_a' & 0 & -M_a' \end{pmatrix} \begin{pmatrix} j_a' & j_a' & L_a' \\ 0 & \nu & -\nu \end{pmatrix} S^*(j_a'j_b'\lambda|S_aS_b) D^{L_a'}_{\nu M_a'}(S_a)^*\Bigg)\Bigg]$$

(Equation continued on following page.)

$$+\left[\Omega(k\ell\ell')^{-1/2}\,(-i)^{\ell+\ell'}\,\alpha(\ell\ell')\sum_{\substack{L_aL_a'L_b\\M_aM_a'M_b}}\sum_{\lambda\lambda'}\alpha^2(\lambda\lambda')\begin{pmatrix}\lambda & \lambda' & \ell'\\0 & 0 & 0\end{pmatrix}\right.$$

$$\times\begin{pmatrix}\lambda & \lambda' & \ell'\\M_a+M_b & -M_a'-M_b & M_a'-M_a\end{pmatrix}\begin{pmatrix}k & \ell & \ell'\\M_a-M_a' & 0 & M_a'-M_a\end{pmatrix}$$

$$\times(-i)^{M_a-M_a'}\,\alpha^2(j_aj_b)\alpha^2(L_b)\alpha^2(L_aL_a')(-1)^{L_a'+M_b}\begin{Bmatrix}q' & q & k\\j_a' & j_a & L_a\\j_a' & j_a & L_a'\end{Bmatrix}\begin{pmatrix}L_a & L_a' & k\\M_a & -M_a' & M_a'-M_a\end{pmatrix}$$

$$\times\sum_{\substack{\nu\mu\\\nu'\mu'}}(-i)^{\nu+\mu-\nu'-\mu'}\begin{pmatrix}j_a & j_a' & L_a\\0 & \nu & -\nu\end{pmatrix}\begin{pmatrix}j_b & j_b' & L_b\\0 & \mu & -\mu\end{pmatrix}\begin{pmatrix}j_a & j_a' & L_a'\\0 & \nu' & -\nu'\end{pmatrix}\begin{pmatrix}j_b & j_b' & L_b\\0 & \mu' & -\mu'\end{pmatrix}$$

$$\times\int d\gamma\gamma^2\int dg'(g')^2\frac{\delta(E)}{gg'}R_{n\ell}(\gamma)R_{n'\ell'}(\gamma')(8\pi^2)^{-4}\iiiint dS_a dS_b dS_a' dS_b'$$

$$\left.\times\; S(j_a'j_b'\lambda|S_aS_b)S^*(j_a'j_b'\lambda'|S_a'S_b')D^{L_a}_{\nu M_a}(S_a)D^{L_b}_{\mu M_b}(S_b)D^{L_a'}_{\nu M_a'}(S_a')^*D^{L_b}_{\mu' M_b}(S_b')^*\right]\Bigg\}\,. \qquad \text{(I.3-11)}$$

In the above expression,

$$\begin{pmatrix}k & \ell & \ell\\0 & 0 & 0\end{pmatrix}\begin{Bmatrix}q' & q & k\\j_a' & j_a' & 0\\j_a' & j_a' & 0\end{Bmatrix}\begin{pmatrix}0 & 0 & k\\0 & 0 & 0\end{pmatrix} = (-1)^{\ell}\,\alpha^{-1}(\ell q)\alpha^{-2}(j_a')\,\delta(qk|q'0)\,, \qquad \text{(I.3-12)}$$

allowing the j_a, j_b, j_a', and j_b' sums to be carried out in the first term in brackets. The λ' sum can be evaluated in the two terms in the second set of brackets,[8,9] yielding $\delta(M_a|0)$ and $\delta(M_a'|0)$.

$$\begin{Bmatrix} q' & q & k \\ j_a' & j_a' & L_a \\ j_a' & j_a' & 0 \end{Bmatrix}\begin{pmatrix} L_a & 0 & k \\ M_a & 0 & -M_a \end{pmatrix} = (-1)^{q-M_a}\,\alpha^{-2}(L_a)\alpha^{-1}(j_a') \times \delta(L_a|k)\begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & k \end{Bmatrix} \tag{I.3-13a}$$

and

$$\begin{Bmatrix} q' & q & k \\ j_a' & j_a' & 0 \\ j_a' & j_a' & L_a' \end{Bmatrix}\begin{pmatrix} 0 & L_a' & k \\ 0 & -M_a' & M_a' \end{pmatrix} = (-1)^{q'-M_a'}\,\alpha^{-2}(L_a')\alpha^{-1}(j_a') \times \delta(L_a'|k)\begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & k \end{Bmatrix}, \tag{I.3-13b}$$

allowing the evaluation of the j_a, j_b, L_a, M_a, L_a', and M_a' sums in the terms in the second set of brackets. The right side of equation (I.3-11) then becomes

$$= \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2}\left\{\sum_{\lambda}\alpha^2(\lambda)\left[\Omega(0qq)^{-1/2}\,\Omega(0\lambda\lambda)^{-1/2}\,\alpha(\ell q)\,\delta(\ell q t k|\ell' q' t' 0)\right.\right.$$

$$\times \int d\gamma\,\frac{\gamma^2}{\mu g}\,R_{n\ell}(\gamma)\,R_{n'\ell}(\gamma) - \sum_{j_a' j_b'}\Omega(kqq')^{-1/2}\,\Omega(k\ell\ell')^{-1/2}$$

$$\times (i)^{q+q'-\ell-\ell'}\,(-1)^{j_a'}\,\alpha^2(j_a')\,\alpha(\ell\ell')(p_{j_a'j_b'})\begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix}\begin{Bmatrix} j_a' & q & j_a' \\ q' & j_a' & k \end{Bmatrix}$$

$$\times \left([\underline{J}]^{(q)}\odot^{q}[\underline{J}]^{(q)}\right)^{1/2}_{j_a'}\left([\underline{J}]^{(q')}\odot^{q'}[\underline{J}]^{(q')}\right)^{1/2}_{j_a'}\,R_t^{(q)}(\varepsilon_{j_a'})\,R_{t'}^{(q')}(\varepsilon_{j_a'})$$

(Equation continued on following page.)

$$\times \int d\gamma \frac{\gamma^2}{\mu g} R_{n\ell}(\gamma)\, R_{n'\ell'}(\gamma) \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a' & j_a' & k \\ 0 & \nu & -\nu \end{pmatrix} (8\pi^2)^{-2} \iint dS_a dS_b$$

$$\times \left\{ S(j_a'j_b'\lambda|S_aS_b) D^k_{\nu 0}(S_a) + (-1)^{q+q'+\nu} S^*(j_a'j_b'\lambda|S_aS_b) D^k_{\nu 0}(S_a)^* \right\} \Big]$$

$$+ \Big[\Omega(kqq')^{-1/2}\, \Omega(k\ell\ell')^{-1/2}\, (i)^{q+q'-\ell-\ell'}\, (-1)^q\, \alpha(\ell\ell')$$

$$\times \sum_{\substack{j_aj_b \\ j_a'j_b'}} \sum_{\substack{L_aL_a'L_b \\ M_aM_a'M_b}} \sum_{\lambda\lambda'} \alpha^2(\lambda\lambda') \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & -M_a'-M_b & M_a'-M_a \end{pmatrix}$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ M_a-M_a' & 0 & M_a'-M_a \end{pmatrix} (-i)^{M_a-M_a'}\, \alpha^2(j_aj_a')\, \alpha(j_bj_b')\, \alpha^2(L_aL_a'L_b)$$

$$\times (p_{j_aj_bj_a'j_b'})^{1/2} \left([\underline{J}]^{(q)} \odot^q [\underline{J}]^{(q)}\right)^{1/2}_{j_a} \left([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')}\right)^{1/2}_{j_a'}$$

$$\times R^{(q)}_t(\varepsilon_{j_a})\, R^{(q')}_{t'}(\varepsilon_{j_a'}) (-1)^{L_a'+M_b} \begin{Bmatrix} q' & q & k \\ j_a' & j_a & L_a \\ j_a' & j_a & L_a' \end{Bmatrix} \begin{pmatrix} L_a & L_a' & k \\ M_a & -M_a' & M_a'-M_a \end{pmatrix}$$

$$\times \sum_{\substack{\nu\mu \\ \nu'\mu'}} (-i)^{\nu+\mu-\nu'-\mu'} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} j_a & j_a' & L_a' \\ 0 & \nu' & -\nu' \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu' & -\mu' \end{pmatrix}$$

$$\times \int d\gamma\gamma^2 \int dg'(g')^2 \frac{\delta(E)}{gg'} R_{n\ell}(\gamma)\, R_{n'\ell'}(\gamma')\, (8\pi^2)^{-4} \iiiint dS_a dS_b dS_a' dS_b'$$

$$\times S(j_a'j_b'\lambda|S_aS_b) S^*(j_a'j_b'\lambda'|S_a'S_b') D^{L_a}_{\nu M_a}(S_a) D^{L_b}_{\mu M_b}(S_b) D^{L_a'}_{\nu' M_a'}(S_a')^* D^{L_b'}_{\mu' M_b}(S_b')^* \Big] \Big\}. \tag{I.3-14}$$

Considering these results,

$$\sigma'\begin{bmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{bmatrix}_k = \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_B T}\right)^{1/2}\Bigg\{\Bigg[\sum_{\lambda}\alpha^2(\lambda)\;\Omega(0qq)^{-1/2}\;\Omega(0\ell\ell)^{-1/2}\;\alpha(\ell q)$$

$$\times\;\delta(\ell qtk|\ell'q't'0)\int d\gamma\,\frac{\gamma^2}{\mu g}\,R_{n\ell}(\gamma)\;R_{n'\ell}(\gamma)\Bigg]$$

$$-\;\Omega(kqq')^{-1/2}\;\Omega(k\ell\ell')^{-1/2}\;(-i)^{q-q'+\ell+\ell'}\;\alpha(\ell\ell')\sum_{\substack{j_a j_b\\ j_a' j_b'}}\;\sum_{\substack{L_a L_a' L_b\\ M_a M_a' M_b}}\;\sum_{\lambda\lambda}\;\sum_{\substack{\nu\mu\\ \nu'\mu'}}$$

$$\times\Bigg[(-i)^{M_a-M_a'}(-i)^{\nu+\mu-\nu'-\mu'}(-1)^{L_a'+M_b}\alpha^2(j_a j_a')\alpha(j_b j_b')(p_{j_a j_b j_a' j_b'})^{1/2}$$

$$\times\;([\underline{J}]^{(q)}\odot\mathcal{A}[\underline{J}]^{(q)})^{1/2}_{j_a}\;([\underline{J}]^{(q')}\odot\mathcal{A}'[\underline{J}]^{(q')})^{1/2}_{j_a'}\;R_t^{(q)}(\varepsilon_{j_a})\;R_{t'}^{(q')}(\varepsilon_{j_a'})$$

$$\times\;\alpha^2(L_a L_a' L_b)\alpha^2(\lambda\lambda')\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda' & \ell'\\ M_a+M_b & -M_a'-M_b & M_a'-M_a\end{pmatrix}\begin{pmatrix}k & \ell & \ell'\\ M_a-M_a' & 0 & M_a'-M_a\end{pmatrix}$$

$$\times\begin{Bmatrix}q' & q & k\\ j_a' & j_a & L_a\\ j_a' & j_a & L_a'\end{Bmatrix}\begin{pmatrix}L_a & L_a' & k\\ M_a & -M_a' & M_a'-M_a\end{pmatrix}\begin{pmatrix}j_a & j_a' & L_a\\ 0 & \nu & -\nu\end{pmatrix}\begin{pmatrix}j_b & j_b' & L_b\\ 0 & \mu & -\mu\end{pmatrix}$$

$$\times\begin{pmatrix}j_a & j_a' & L_a'\\ 0 & \nu' & -\nu'\end{pmatrix}\begin{pmatrix}j_b & j_b' & L_b\\ 0 & \mu' & -\mu'\end{pmatrix}\int d\gamma\gamma^2\int dg'(g')^2\,\frac{\delta(E)}{gg'}\,R_{n\ell}(\gamma)R_{n'\ell'}(\gamma')$$

$$\times\;(8\pi^2)^{-4}\iiiint dS_a dS_b dS_a' dS_b'\;S(j_a' j_b'\lambda|S_a S_b)\;S^*(j_a' j_b'\lambda'|S_a' S_b')$$

$$\times\;D^{L_a}_{\nu M_a}(S_a)\;D^{L_b}_{\mu M_b}(S_t)\;D^{L_a'}_{\nu' M_a'}(S_a')^*D^{L_b}_{\mu' M_b}(S_b')^*\Bigg]\Bigg\}\,. \qquad (I.3\text{-}15)$$

Before proceeding to the reduction of this collision integral, it is useful to integrate over the energy delta function appearing in the term quadratic in S. When this is done,

$$\alpha^2(j_a j_a')\alpha(j_b j_b')(p_{j_a j_b j_a' j_b'})^{1/2} \int d\gamma\gamma^2 \int dg'(g')^2 \frac{\delta(E)}{\partial g'} R_{n\ell}(\gamma)R_{n'\ell'}(\gamma')$$

$$= \alpha^3(j_a)\alpha(j_a')\alpha^2(j_b)(p_{j_a' j_b'}) \left[\frac{\Gamma(n+1)\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2} \frac{2}{\sqrt{2\mu k_B T}}$$

$$\times \int d\gamma[\gamma^2 + (\varepsilon_{j_a'} + \varepsilon_{j_b'} - \varepsilon_{j_a} - \varepsilon_{j_b})]^{\ell/2} \gamma^{\ell+1} \quad e^{-\gamma^2}$$

$$\times L_n^{\ell+1/2}(\gamma^2 + \varepsilon_{j_a'} + \varepsilon_{j_b'} - \varepsilon_{j_a} - \varepsilon_{j_b})L_{n'}^{\ell'+1/2}(\gamma^2) \ . \qquad \text{(I.3-16)}$$

Equation (I.3-15) can now be written

$$\sigma'\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\left\{\left[\sum_\lambda \alpha^2(\lambda)\ \Omega(0qq)^{-1/2}\ \Omega(0\ell\ell)^{-1/2}\ \alpha(\ell q)\right.\right.$$

$$\left. \times\ \delta(\ell qtk|\ell'q't'0) \int d\gamma\gamma\ R_{n\ell}(\gamma)R_{n'\ell}(\gamma)\right]$$

$$-\ 2\Omega(kqq')^{-1/2}\ \Omega(k\ell\ell')^{-1/2}\ (-i)^{q-q'+\ell+\ell'}\ \alpha(\ell\ell') \sum_{\substack{j_a j_b\\ j_a' j_b'}} \sum_{\substack{L_a L_a' L_b\\ M_a M_a' M_b}} \sum_{\substack{\lambda\lambda'\\ \nu'\mu'}}$$

$$\times \left[(-i)^{M_a - M_a' - \nu' - \mu'} (-1)^{L_a' + M_b} \alpha^3(j_a)\alpha^2(j_b)\alpha(j_a')\right.$$

(Equation continued on following page.)

$$\times\ (p_{j_a' j_b'})([\underline{J}]^{(q)} \odot^{q} [\underline{J}]^{(q)})^{1/2}_{j_a}\ ([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')})^{1/2}_{j_a'}$$

$$\times\ \alpha^2(L_a L_a' L_b)\ \alpha^2(\lambda\lambda') \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & -M_a'-M_b & M_a'-M_a \end{pmatrix}$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ M_a-M_a' & 0 & M_a'-M_a \end{pmatrix} \begin{Bmatrix} q' & q & k \\ j_a' & j_a & L_a \\ j_a' & j_a & L_a' \end{Bmatrix} \begin{pmatrix} L_a & L_a' & k \\ M_a & -M_a' & M_a'-M_a \end{pmatrix} R_{t'}^{(q')}(\varepsilon_{j_a'})$$

$$\times \begin{pmatrix} j_a & j_a' & L_a' \\ 0 & \nu' & -\nu' \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} \left[\frac{\Gamma(n+1)\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2}$$

$$\times\ (8\pi^2)^{-4} \iiiint dS_a dS_b dS_a' dS_b'\ S(j_a' j_b' \lambda | S_a S_b)\ S^{*}(j_a' j_b' \lambda' | S_a' S_b')$$

$$\times\ D^{L_a'}_{\nu' M_a'}(S_a')^{*}\ D^{L_b}_{\mu' M_b}(S_b')^{*}\ R_t^{(q)}(\varepsilon_{j_a}) \int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n'}^{\ell'+1/2}(\gamma^2)$$

$$\times\ [\gamma^2 + \varepsilon_{j_a'} + \varepsilon_{j_b'} - \varepsilon_{j_a} - \varepsilon_{j_b}]^{\ell/2}\ L_n^{\ell+1/2}(\gamma^2 + \varepsilon_{j_a'} + \varepsilon_{j_b'} - \varepsilon_{j_a} - \varepsilon_{j_b})$$

$$\times \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\ D^{L_b}_{\mu M_b}(S_b) \Bigg] \Bigg\}\ , \qquad (I.3\text{-}17)$$

an expression that provides a convenient starting point for the general reduction to be accomplished in the next section.

I.4 Reduction of the $\mathcal{J}'\begin{bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{bmatrix}_k$ Collision Integrals

In this section, equation (I.3-17) is reduced to a summation over eight indices and an integration over six angles, in contrast to its present form requiring a sixteen-fold summation and twelve-fold angle integration. The reduction is made possible by the introduction of certain operators, as well as the explicit summation over several indices.

In Reference 10, it is shown that

$$[\varepsilon_{j_a'} - \varepsilon_{j_a}] \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) = -\frac{1}{2I_a k_B T} K^{(a)*}$$

$$\times \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) , \qquad \text{(I.4-1a)}$$

$K^{(a)*}$ being defined in that same reference. Repeated application of the operator, $[-\frac{1}{2I_a k_B T} K^{(a)*}]$, to both sides of (I.4-1a) yields

$$[\varepsilon_{j_a'} - \varepsilon_{j_a}]^m \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) = [-\frac{1}{2I_a k_B T} K^{(a)*}]^m$$

$$\times \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) , \qquad \text{(I.4-1b)}$$

$$m = \text{integer},$$

and as a consequence,

$$[\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b}]^m \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) D^{L_b}_{\mu M_b}(S_b)$$

$$= \left[-\frac{1}{k_B T}\left(\frac{K^{(a)*}}{2I_a} + \frac{K^{(b)*}}{2I_b}\right)\right]^m \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix}$$

$$\times D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b) \,, \qquad m = \text{integer} \,. \qquad \text{(I.4-1c)}$$

Remembering that $R_t^{(q)}(\varepsilon_{j_a})$ is a Wang Chang-Uhlenbeck polynomial, it is possible to write

$$R_t^{(q)}(\varepsilon_{j_a}) \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)$$

$$= R_t^{(q)}\left(\varepsilon_{j_a'} + \frac{1}{2I_a k_B T} K^{(a)*}\right) \sum_{\nu} (-i)^{\nu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) \,. \qquad \text{(I.4-2a)}$$

Moreover, since $[\gamma^2+\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b}]^{\ell/2}$ and $L_n^{\ell+1/2}(\gamma^2+\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b})$ can be expanded in power series involving integer powers of $(\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b})$,

$$\left\{[\gamma^2+\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b}]^{\ell/2}\, L_n^{\ell+1/2}(\gamma^2+\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b})\right\}\sum_{\nu\mu}(-i)^{\nu+\mu}$$

$$\times\begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix}\begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)$$

$$= \left\{[\gamma^2 - \frac{1}{k_BT}K^*]^{\ell/2}\, L_n^{\ell+1/2}(\gamma^2 - \frac{1}{k_BT}K^*)\right\}\sum_{\nu\mu}(-i)^{\nu+\mu}$$

$$\times\begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix}\begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)\ , \qquad (1.4\text{-}2b)$$

in which $K^* \equiv (K^{(a)*}/2I_a) + (K^{(b)*}/2I_b)$. Finally,

$$R_t^{(q)}(\varepsilon_{j_a})[\gamma^2+\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b}]^{\ell/2}\, L_n^{\ell+1/2}(\gamma^2+\varepsilon_{j_a'}+\varepsilon_{j_b'}-\varepsilon_{j_a}-\varepsilon_{j_b})$$

$$\times\sum_{\nu\mu}(-i)^{\nu+\mu}\begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix}\begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)$$

$$= C_{ab}(\ell qnt)\sum_{\nu\mu}(-i)^{\nu+\mu}\begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix}\begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)\ , \qquad (1.4\text{-}2c)$$

where the operator is defined as

$$C_{ab}(\ell qnt) \equiv R_t^{(q)}(\varepsilon_{j_a'} + \frac{1}{2I_ak_BT}K^{(a)})[\gamma^2 - \frac{1}{k_BT}K^*]^{\ell/2} \qquad (1.4\text{-}2d)$$

$$L_n^{\ell+1/2}(\gamma^2 - \frac{1}{k_BT}K^*)\ .$$

Making use of the fact that $\kappa^{(a)*}$ and $\kappa^{(b)*}$ are hermitian,[10]

$$\iint dS_a dS_b \; S(j_a' j_b' \lambda | S_a S_b) \int d\gamma \; \gamma^{\ell+1} \; e^{-\gamma^2} \; L_{n'}^{\ell'+1/2}(\gamma^2) \; C_{ab}(\ell q n t)$$

$$\times \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) \; D^{L_b}_{\mu M_b}(S_b)$$

$$= \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} \int d\gamma \; \gamma^{\ell+1} \; e^{-\gamma^2} \; L_{n'}^{\ell'+1/2}(\gamma^2)$$

$$\times \iint dS_a dS_b \; [C^{*}_{ab}(\ell q n t) \; S(j_a' j_b' \lambda | S_a S_b)] \; D^{L_a}_{\nu M_a}(S_a) \; D^{L_b}_{\mu M_b}(S_b) \; . \qquad (I.4\text{-}3)$$

This allows equation (1.3-17) to be written

$$\omega' \begin{bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{bmatrix}_k = \frac{\hbar^2 \pi^{3/2}}{4\mu k_B T} \left\{ \left[\sum_\lambda \alpha^2(\lambda) \; \Omega(0qq)^{-1/2} \; \Omega(0\ell\ell)^{-1/2} \; \alpha(\ell q) \right. \right.$$

$$\times \; \delta(\ell q t k | \ell' q' t' 0) \int d\gamma \; R_{n\ell}(\gamma) R_{n'\ell}(\gamma)]$$

$$- \; 2\Omega(kqq')^{-1/2} \; \Omega(k\ell\ell')^{-1/2} \; (-i)^{q-q'+\ell+\ell'} \; \alpha(\ell\ell') \sum_{\substack{j_a j_b \\ j_a' j_b'}} \; \sum_{\substack{L_a L_a' L_b \\ M_a M_a' M_b}} \; \sum_{\lambda\lambda'} \; \sum_{\substack{\nu\mu \\ \nu'\mu'}}$$

$$\times \Big[(-i)^{M_a - M_a'} \; (-i)^{\nu+\mu-\nu'-\mu'} \; (-1)^{L_a'+M_b} \; \alpha^3(j_a) \; \alpha^2(j_b) \; \alpha(j_a')$$

(Equation continued on following page.)

$$\times\ (p_{j'_a j'_b})\left([\underline{J}]^{(q)}\mathcal{P}[\underline{J}]^{(q)}\right)^{1/2}_{j_a}\left([\underline{J}]^{(q')}\mathcal{P}'[\underline{J}]^{(q')}\right)^{1/2}_{j'_a}\ \alpha^2(L_a L'_a L_b)\ \alpha^2(\lambda\lambda')$$

$$\times\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda' & \ell'\\ M_a+M_b & -M'_a-M_b & M'_a-M_a\end{pmatrix}\begin{pmatrix}k & \ell & \ell'\\ M_a-M'_a & 0 & M'_a-M_a\end{pmatrix}\begin{Bmatrix}q' & q & k\\ j'_a & j_a & L_a\\ j'_a & j_a & L'_a\end{Bmatrix}$$

$$\times\begin{pmatrix}L_a & L'_a & k\\ M_a & -M'_a & M'_a-M_a\end{pmatrix}\begin{pmatrix}j_a & j'_a & L_a\\ 0 & \nu & -\nu\end{pmatrix}\begin{pmatrix}j_a & j'_a & L'_a\\ 0 & \nu' & -\nu'\end{pmatrix}\begin{pmatrix}j_b & j'_b & L_b\\ 0 & \mu & -\mu\end{pmatrix}\begin{pmatrix}j_b & j'_b & L_b\\ 0 & \mu' & -\mu'\end{pmatrix}$$

$$\times\left[\frac{\Gamma(n+1)\ \Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2}\ (8\pi^2)^{-4}\int d\gamma\,\gamma^{\ell+1}\ e^{-\gamma}\ L_{n'}^{\ell'+1/2}(\gamma)R_{t'}^{(q')}(\varepsilon_{j'_a})$$

$$\times\iiiint dS_a dS_b dS'_a dS'_b\ [C^{*}_{ab}(\ell qnt)\ S(j'_a j'_b\lambda|S_a S_b)]$$

$$\times S^{*}(j'_a j'_b\lambda'|S'_a S'_b)\ D^{L_a}_{\nu M_a}(S_a)\ D^{L_b}_{\mu M_b}(S_b)\ D^{L'_a}_{\nu' M_a}(S'_a)^{*}\ D^{L_b}_{\mu' M_b}(S'_b)^{*}\Big]\Big\}\ . \tag{I.4-4}$$

Now, the j_b sum can be evaluated,[8,9]

$$\sum_{j_b}\alpha^2(j_b)\begin{pmatrix}j_b & j'_b & L_b\\ 0 & \mu & -\mu\end{pmatrix}\begin{pmatrix}j_b & j'_b & L_b\\ 0 & \mu & -\mu'\end{pmatrix} = \delta_{\mu\mu'}\ , \tag{I.4-5}$$

and the 9-j symbol expanded,[8]

$$\begin{Bmatrix} q' & q & k \\ j_a' & j_a & L_a \\ j_a' & j_a & L_a' \end{Bmatrix} \begin{pmatrix} L_a & L_a' & k \\ M_a & -M_a' & M_a'-M_a \end{pmatrix} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_a & j_a' & L_a' \\ 0 & \nu' & -\nu' \end{pmatrix}$$

$$= \sum_{\substack{\kappa\,\mu_1\mu_2, \\ \mu_1'\mu_2', \\ \mu_1''\mu_2''}} a^2(\kappa)(-1)^{\kappa+j_a+j_a'+\mu_1+\mu_1'+\mu_1''+M_a} \begin{pmatrix} j_a & \kappa & j_a' \\ 0 & \mu_2 & -\mu_2 \end{pmatrix} \begin{pmatrix} q' & j_a' & j_a' \\ -\mu_1 & \nu' & \mu_2 \end{pmatrix}$$

$$\times \begin{pmatrix} q' & \kappa & L_a' \\ \mu_1 & -\mu_2 & -\nu' \end{pmatrix} \begin{pmatrix} j_a & q & j_a \\ 0 & \mu_2' & -\mu_2' \end{pmatrix} \begin{pmatrix} \kappa & j_a' & j_a \\ -\mu_1' & \nu & \mu_2' \end{pmatrix} \begin{pmatrix} \kappa & q & L_a \\ \mu_1' & -\mu_2' & -\nu \end{pmatrix}$$

$$\times \begin{pmatrix} L_a & q & \kappa \\ M_a & \mu_2'' & -M_a-\mu_2'' \end{pmatrix} \begin{pmatrix} q' & L_a' & \kappa \\ -\mu_1'' & -M_a' & M_a+\mu_2'' \end{pmatrix} \begin{pmatrix} q' & q & k \\ \mu_1'' & -\mu_2'' & M_a'-M_a \end{pmatrix}, \tag{I.4-6}$$

to yield

$$\sigma'\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\left\{\left[\sum_{\lambda} \alpha^2(\lambda)\Omega(0qq)^{-1/2}\Omega(0\ell\ell)^{-1/2}\,\alpha(\ell q)\right.\right.$$

$$\times\ \delta(\ell q t k|\ell' q' t' 0)\int d\gamma\ \gamma R_{n\ell}(\gamma)\ R_{n'\ell}(\gamma)\Big]$$

$$-\ 2\Omega(kqq')^{-1/2}\Omega(k\ell\ell')^{-1/2}(-i)^{q-q'+\ell+\ell'}\ \alpha(\ell\ell')\left[\frac{\Gamma(n+1)\ \Gamma(n'+1)}{\Gamma(n+\ell+\frac{1}{2})\Gamma(n'+\ell'+\frac{1}{2})}\right]^{1/2}$$

$$\times\ (8\pi^2)^{-4}\sum_{\substack{j_a j_a' j_b'\\ \lambda\lambda'}}\ \sum_{\substack{L_b M_b M_a M_a'\\ \nu\mu\nu'}}\ \sum_{\substack{\kappa\mu_1\mu_2\\ \mu_1'\mu_2'\\ \mu_1''\mu_2''}}(-i)^{M_a-M_a'+\cdots}$$

$$\times\ (-1)^{\kappa+j_a+j_a'+\mu_1+\mu_1'+\mu_1''+M_a+M_b}\ \alpha^3(j_a)\alpha(j_a')(p_{j_a'j_b'})([\underline{J}]^{(q)}\odot\mathfrak{q}[\underline{J}]^{(q)})_{j_a}^{1/2}$$

$$\times\ ([\underline{J}]^{(q')}\odot\mathfrak{q}'[\underline{J}]^{(q')})_{j_a'}^{1/2}\ \alpha^2(\kappa L_b)\ \alpha^2(\lambda\lambda')$$

$$\times\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda' & \ell'\\ M_a+M_b & -M_a'-M_b & M_a'-M_a\end{pmatrix}\begin{pmatrix}k & \ell & \ell'\\ M_a-M_a' & 0 & M_a'-M_a\end{pmatrix}\begin{pmatrix}j_a & \kappa & j_a'\\ 0 & \mu_2 & -\mu_2\end{pmatrix}$$

$$\times\begin{pmatrix}q' & j_a' & j_a'\\ -\mu_1 & \nu' & \mu_2\end{pmatrix}\begin{pmatrix}j_a & q & j_a\\ 0 & \mu_2' & -\mu_2'\end{pmatrix}\begin{pmatrix}\kappa & j_a' & j_a\\ -\mu_1' & \nu & \mu_2'\end{pmatrix}\begin{pmatrix}q' & q & k\\ \mu_1'' & -\mu_2'' & M_a'-M_a\end{pmatrix}$$

$$\times\int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n'}^{\ell'+1/2}(\gamma^2)R_{t'}^{(q')}(\varepsilon_{j_a'})\iiiint dS_a dS_b dS_a' dS_b'$$

$$\times\ [C_{ab}^{*}(\ell qnt)\ S(j_a'j_b'\lambda|S_aS_b)]\ S^{*}(j_a'j_b'\lambda'|S_a'S_b')D_{\mu M_b}^{L_b}(S_b)\ D_{\mu M_b}^{L_b}(S_b')^{*}$$

(Equation continued on following page.)

$$\times \left\{ \sum_{L_a} \alpha^2(L_a) \begin{pmatrix} \kappa & q & L_a \\ \mu_1' & -\mu_2' & -\nu \end{pmatrix} \begin{pmatrix} L_a & q & \kappa \\ M_a & \mu_2'' & -M_a-\mu_2'' \end{pmatrix} D^{L_a}_{\nu M_a}(S_a) \right\}$$

$$\times \left\{ \sum_{L_a'} (-1)^{L_a'} \alpha^2(L_a') \begin{pmatrix} q' & \kappa & L_a' \\ \mu_1 & -\mu_2 & -\nu' \end{pmatrix} \begin{pmatrix} q & L_a' & \kappa \\ -\mu_1' & -M_a' & M_a+\mu_2'' \end{pmatrix} D^{L_a'}_{\nu' M_a'}(S_a')^* \right\} \} .$$

(I.4-7)

Using Ref. 8, the sums over L_a and L_a' can be carried out,

$$\sum_{L_a} \alpha^2(L_a) \begin{pmatrix} \kappa & q & L_a \\ \mu_1' & -\mu_2' & -\nu \end{pmatrix} \begin{pmatrix} L_a & q & \kappa \\ M_a & \mu_2'' & -M_a-\mu_2'' \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)$$

$$= (-1)^{\nu+M_a} \delta_{\nu,\mu_1'-\mu_2'} D^{\kappa}_{\mu_1',M_a+\mu_2''}(S_a) \quad D^{q}_{-\mu_2',-\mu_2''}(S_a) ,$$

(I.4-8a)

and

$$\sum_{L_a'} (-1)^{L_a'} \alpha^2(L_a') \begin{pmatrix} q' & \kappa & L_a' \\ \mu_1 & -\mu_2 & -\nu' \end{pmatrix} \begin{pmatrix} q' & L_a' & \kappa \\ -\mu_1'' & -M_a' & M_a+\mu_2'' \end{pmatrix} D^{L_a'}_{\nu' M_a'}(S_a')^*$$

$$= (-1)^{q'+\kappa} \delta_{\nu',\mu_1-\mu_2} \delta_{M_a',M_a-\mu_1''+\mu_2''} D^{q'}_{-\mu_1,\mu_1''}(S_a') \, D^{\kappa}_{\mu_2,-M_a-\mu_2''}(S_a') ,$$

(I.4-8b)

followed by the sums over ν, ν', and M_a'. After relabelling indices,

$$\sigma'\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\Big\{\Big[\sum_{\lambda}\alpha^2(\lambda)\Omega(0qq)^{-1/2}\Omega(0\ell\ell)^{-1/2}\,\alpha(\ell q)$$

$$\times\,\delta(\ell q t k|\ell' q' t' 0)\int d\gamma\,\gamma\,R_{n\ell}(\gamma)\,R_{n'\ell}(\gamma)\Big]$$

$$-\,2\Omega(kqq')^{-1/2}\,\Omega(k\ell\ell')^{-1/2}\,(i)^{q-q'+\ell+\ell'}\,\alpha(\ell\ell')\left[\frac{\Gamma(n+1)\,\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2}$$

$$\times\,(8\pi^2)^{-4}\sum_{\substack{j_a j_a' j_b'\\ \lambda\lambda' L_b \kappa}}\Big[\alpha^2(\lambda\lambda')\alpha^2(L_b\kappa)\alpha^3(j_a)\alpha(j_a')(p_{j_a' j_b'})$$

$$\times\,([\underline{J}]^{(q)}\odot^{q}[\underline{J}]^{(q)})_{j_a}^{1/2}\,([\underline{J}]^{(q')}\odot^{q'}[\underline{J}]^{(q')})_{j_a'}^{1/2}$$

$$\sum_{\substack{\beta\mu\mu_1\mu_2\\ \mu_1'\mu_2'\mu_1''\mu_2''\mu_3''}}(-i)^{\mu_1-\mu_1'-\mu_2+\mu_2'+\mu_3''-\mu_2''}\,(-1)^{j_a+j_a'+\mu+\mu_2+\mu_1'+\mu_1''}$$

$$\times\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda' & \ell'\\ -\mu & \mu+\mu_2'-\mu_3'' & \mu_3''-\mu_2''\end{pmatrix}\begin{pmatrix}\ell & k & \ell'\\ 0 & \mu_2''-\mu_3'' & \mu_3''-\mu_2''\end{pmatrix}$$

$$\times\begin{pmatrix}j_a & q & j_a\\ 0 & \mu_2 & -\mu_2\end{pmatrix}\begin{pmatrix}\kappa & j_a' & j_a\\ -\mu_1 & \mu_1-\mu_2 & \mu_2\end{pmatrix}\begin{pmatrix}j_a & \kappa & j_a'\\ 0 & \mu_2' & -\mu_2'\end{pmatrix}\begin{pmatrix}q' & j_a' & j_a'\\ -\mu_1' & \mu_1'-\mu_2' & \mu_2'\end{pmatrix}$$

$$\times\begin{pmatrix}k & q & q'\\ \mu_3''-\mu_2'' & \mu_2'' & -\mu_3''\end{pmatrix}\int d\gamma\,\gamma^{\ell+1}\,e^{-\gamma^2}\,L_{n'}^{\ell'+1/2}(\gamma^2)\,R_{t'}^{(q')}(\epsilon_{j_a'})$$

$$\times\iint dS_a\,dS_b\,[C^{*}_{ab}(\ell q n t)S(j_a' j_b' \lambda|S_a S_b)]\,D^{\kappa}_{\mu_1-\mu_1''}(S_a)\,D^{q}_{-\mu_2\mu_2''}(S_a)$$

(Equation continued on following page.)

$$\times D^{L_b}_{\beta,-\mu+\mu_1''-\mu_2''}(S_b) \iint dS_a' dS_b'\, S^{\star}(j_a'j_b'\lambda'|S_a'S_b')\, D^{\kappa}_{\mu_2'\mu_1''}(S_a')$$

$$\times D^{q'}_{-\mu_1'-\mu_2''}(S_a')\, D^{L_b}_{\beta,-\mu+\mu_1''-\mu_2''}(S_b')^{\star}\Big]\Big\} . \qquad (I.4\text{-}9)$$

At this point it is convenient to introduce a compact notation for the j_a summation:

$$I(q\mu_2;\kappa j_a'\mu_1\mu_2') = \sum_{j_a} (-1)^{j_a}\, \alpha^3(j_a)([\underline{J}]^{(q)} \odot \mathcal{A}[\underline{J}]^{(q)})^{1/2}_{j_a}$$

$$\times \begin{pmatrix} j_a & q & j_a \\ 0 & \mu_2 & -\mu_2 \end{pmatrix} \begin{pmatrix} \kappa & j_a' & j_a \\ -\mu_1 & \mu_1-\mu_2 & \mu_2 \end{pmatrix} \begin{pmatrix} \kappa & j_a' & j_a \\ \mu_2' & -\mu_2' & 0 \end{pmatrix} , \qquad (I.4\text{-}10a)$$

as well as two operators defined on the S_aS_b and S_a' angle spaces, respectively, by the following eigenvalue relations:

$$\ell_{ab}(\lambda\lambda'\ell':M_a-\beta) D^{L_a}_{\nu M_a}(S_a) D^{L_b}_{\mu M_b}(S_b) = (-1)^{-\hbar^{-1}M_3}$$

$$\cdot \begin{pmatrix} \lambda & \lambda' & \ell' \\ \hbar^{-1}M_3 & -\hbar^{-1}M_3+\beta-M_a & M_a-\beta \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)$$

$$= (-1)^{M_a+M_b} \begin{pmatrix} \lambda & \lambda' & \ell' \\ -M_a-M_b & M_b+\beta & M_a-\beta \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b) \qquad (I.4\text{-}10b)$$

and

$$\mathcal{E}_{a'}(q'j_a';\mu_1')D^{L_a'}_{\nu' M_a'}(S_a') = (-1)^{j_a' - \hbar^{-1}\mathcal{L}_3^{(a')}}$$

$$\times \begin{pmatrix} q' & j_a' & j_a' \\ \mu_1' & \hbar^{-1}\mathcal{L}_3^{(a')}-\mu_1' & -\hbar^{-1}\mathcal{L}_3^{(a')} \end{pmatrix} D^{L_a'}_{\nu' M_a'}(S_a')$$

$$= (-1)^{j_a'-\nu'} \begin{pmatrix} q' & j_a' & j_a' \\ \mu_1' & \nu'-\mu_1' & -\nu' \end{pmatrix} D^{L_a'}_{\nu' M_a'}(S_a') , \qquad \text{(I.4-10c)}$$

where $\mathcal{M}_3$ and $\mathcal{L}_3^{(a')}$ are both defined in Ref. 10. Now

$$\mathcal{E}_{ab}(\lambda\lambda'\ell';\mu_3''-\mu_2'')[D^{\kappa}_{\mu_1-\mu_1''}(S_a)D^{q}_{-\mu_2\mu_2''}(S_a)D^{L_b}_{\beta,-\mu+\mu_1''-\mu_2''}(S_b)]$$

$$= (-1)^{\mu} \begin{pmatrix} \lambda & \lambda' & \ell' \\ -\mu & \mu+\mu_2''-\mu_3'' & \mu_3''-\mu_2'' \end{pmatrix} [D^{\kappa}_{\mu_1-\mu_1''}(S_a)D^{q}_{-\mu_2\mu_2''}(S_a)$$

$$\times D^{L_b}_{\beta,-\mu+\mu_1''-\mu_2''}(S_b)] . \qquad \text{(I.4-11)}$$

If the 3-j symbols on the RHS of equations (I.4-10b) and (I.4-10c) are expanded,[8,9] they, along with the phases, become polynomials in (M_a+M_b) and ν', respectively. Similarly, the operators $\mathcal{E}_{ab}$ and $\mathcal{E}_{a'}$ can be expanded as polynomials in $\mathcal{M}_3$ and $\mathcal{L}_3^{(a')}$. It should be noted that K and $\mathcal{M}_3$ commute, while K and $\mathcal{L}_3^{(a')}$ do not. Thus K commutes with $\mathcal{E}_{ab}(\lambda\lambda'\ell';\mu_3''-\mu_2'')$ but not with $\mathcal{E}_{a'}(q'j_a';\mu_1')$.

Once the value of q has been specified, the $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$ sums can be evaluated using recursion relations among the 3-j coefficients. Values for $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$ are given in Appendix I.A for $q=0,1$, and 2. These are sufficient to evaluate transport properties in an applied field.[1]

Introducing the above and making use of the fact that M_3 and $L_3^{(a')}$, and consequently $E_{ab}(\lambda\lambda'\ell';\mu_3''-\mu_2'')$ and $E_{a'}(q'j_a';\mu_1')$, are hermitian,[10] it is possible to write

$$\sigma'\begin{bmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{bmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\Bigg\{\Big[\sum_{\lambda}\alpha^2(\lambda)\Omega(0qq)^{-1/2}\Omega(0\ell\ell)^{-1/2}\,\alpha(\ell q)$$

$$\times\,\delta(\ell q t k|\ell' q' t' 0)\int d\gamma\,\gamma\,R_{n\ell}(\gamma)\,R_{n'\ell}(\gamma)\Big]$$

$$-\,2\Omega(kqq')^{-1/2}\Omega(k\ell\ell')^{-1/2}(i)^{q-q'+\ell+\ell'}\,\alpha(\ell\ell')\left[\frac{\Gamma(n+1)\;\Gamma(n'+1)}{\Gamma(n+\ell+\frac{3}{2})\Gamma(n'+\ell'+\frac{3}{2})}\right]^{1/2}$$

$$\times\,(8\pi^2)^{-4}\sum_{\substack{j_a'j_b'\\ \lambda\lambda'\\ L_b\kappa}}\big[\alpha^2(\lambda\lambda')\alpha^2(L_b\kappa)\alpha(j_a')(p_{j_a'j_b'})([\underline{J}]^{(q')}\odot^{q'}[\underline{J}]^{(q')})^{1/2}_{j_a'}$$

$$\times\sum_{\substack{\beta\mu\mu_1\mu_2\\ \mu_1'\mu_2'\mu_1''\mu_2''\mu_3''}}(-i)^{\mu_1-\mu_1'-\mu_2+\mu_2'+\mu_3''-\mu_2''}(-1)^{\mu_2+\mu_2'+\mu_1'+\mu_1''}$$

$$\times\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & k & \ell'\\ 0 & \mu_2''-\mu_3'' & \mu_3''-\mu_2''\end{pmatrix}\begin{pmatrix}k & q & q'\\ \mu_3''-\mu_2'' & \mu_2'' & -\mu_3''\end{pmatrix}$$

(Equation continued on following page.)

$$\times\ I(q\mu_2;\kappa j_a'\mu_1\mu_2')R_{t'}^{(q')}(\epsilon_{j_a'}) \int d\gamma\ \gamma^{\lambda+1}\ e^{-\gamma^2}\ L_{n'}^{\ell'+\frac{1}{2}}(\gamma^2)$$

$$\times \left\{\iiint dS_a dS_b[E_{ab}^{*}(\lambda\lambda'\ell';\mu_3''-\mu_2'')C_{ab}^{*}(\ell qnt)S(j_a'j_b'\lambda|S_aS_b)]D_{\mu_1-\mu_1''}^{\kappa}(S_a)\right.$$

$$\left.\times\ D_{-\mu_2\mu_2''}^{q}(S_a)\ D_{\beta,-\mu}^{L_b}(S_b)\right\}$$

$$\times \left\{\iiint dS_a'dS_b'[E_{a'}^{*}(q'j_a';\mu_1')D_{-\mu_1'-\mu_3''}^{q'}(S_a')S^{*}(j_a'j_b'\lambda'|S_a'S_b')]\right.$$

$$\left.\times\ D_{\mu_2'\mu_1''}^{\kappa}(S_a')\ D_{\beta,-\mu}^{L_b}(S_b')^{*}\right]\Bigg\}\ . \qquad (I.4\text{-}12)$$

In order to proceed beyond the above expression, it is useful to introduce another operator, $I_{a'}(q\mu_2)$, defined by the relation

$$I_{a'}^{+*}(q\mu_2)\ f(S_a') = (8\pi^2)^{-1} \sum_{\substack{\kappa\mu_1 \\ \mu_1''\mu_2'}} D_{-\mu_1\mu_1''}^{\kappa}(S_a')^{*}\ (i)^{\mu_1+\mu_2'} \qquad (I.4\text{-}13a)$$

$$\times\ I(q\mu_2;\kappa j_a'\mu_1\mu_2') \int dS_a''\ D_{\mu_2'\mu_1''}^{\kappa}(S_a'')\ f(S_a'')\ ,$$

where $f(S_a')$ is an arbitrary function in the S_a' angle space. As a consequence of (I.4-13a),

$$\sum_{\mu_2'} (i)^{\mu_1+\mu_2'}\ I(q\mu_2;\kappa j_a'\mu_1\mu_2') \int dS_a'\ f(S_a')D_{\mu_2'\mu_1''}^{\kappa}(S_a')$$

$$= \int dS_a'\ D_{-\mu_1\mu_1''}^{\kappa}(S_a')I_{a'}^{+*}(q\mu_2)\ f(S_a') = \int dS_a'\ f(S_a')I_{a'}(q\mu_2)D_{-\mu_1\mu_1''}^{\kappa}(S_a'),$$

$$(I.4\text{-}13b)$$

taking the adjoint of $I^{\dagger *}_{a'}(q\mu_2)$. The above expression can be used to determine $I_{a'}(q\mu_2)$ for a given $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$. The $I_{a'}(q\mu_2)$ corresponding to the $q = 0,1,$ and 2 values of $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$ are also given in Appendix I.A.

The $I_{a'}(q\mu_2)$ operators isolate all the explicit dependence on the indices κ and μ_1 appearing in the $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$ in the rotation matrix elements, $D^{\kappa}_{-\mu_1\mu_1''}(S_a')$, instead. Equation (I.4-12) can now be written as

$$
\begin{aligned}
\sigma'\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T} & \Big\{ \Big[\sum_{\lambda} \alpha^2(\lambda)\,\Omega(0qq)^{-1/2}\,\Omega(0\ell\ell)^{-1/2}\,\alpha(\ell q) \\
& \times \delta(\lambda qtk|\ell'q't'0) \int d\gamma\, \gamma\, R_{n\ell}(\gamma)\, R_{n'\ell}(\gamma)\Big] \\
& - 2\Omega(kqq')^{-1/2}\,\Omega(k\ell\ell')^{-1/2}\,(i)^{q-q'+\ell+\ell'}\,\alpha^2(\ell\ell') \left[\frac{\Gamma(n+1)\;\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\,\Gamma(n'+\ell'+3/2)}\right]^{1/2} \\
& \times (8\pi^2)^{-4} \sum_{\substack{j_a' j_b' \\ \lambda\lambda'}} \Big[\alpha^2(\lambda\lambda')\,\alpha(j_a')\,(p_{j_a'j_b'})\,\big([\underline{J}]^{(q')}\epsilon^{q'}[\underline{J}]^{(q')}\big)^{1/2}_{j_a'} \\
& \times \sum_{\substack{\mu_2\mu_1 \\ \mu_2''\mu_3''}} (-i)^{\mu_1'+\mu_2+\mu_3''-\mu_2''} \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & k & \ell' \\ 0 & \mu_2''-\mu_3'' & \mu_3''-\mu_2'' \end{pmatrix} \\
& \times \begin{pmatrix} k & q & q' \\ \mu_3''-\mu_2'' & \mu_2'' & -\mu_3'' \end{pmatrix} R^{(q')}_{t'}(\epsilon_{j_a'}) \int d\gamma\, \gamma^{\ell+1}\, e^{-\gamma^2}\, L^{\ell'+1/2}_{n'}(\gamma^2)
\end{aligned}
$$

(Equation continued on following page.)

$$\times \iiiint dS_a dS_b dS_a' dS_b' [\mathcal{E}^{\star}_{ab}(\lambda\lambda'\ell';\mu_3''-\mu_2'') C^{\star}_{ab}(\ell q n t) S(j_a' j_b' \lambda | S_a S_b)]$$

$$\times D^{q}_{-\mu_2 \mu_2''}(S_a) [\mathcal{I}^{\dagger\star}_{a'}(q\mu_2) \mathcal{E}^{\star}_{a'}(q' j_a'; \mu_1') D^{q'}_{-\mu_1', -\mu_3''}(S_a') S^{\star}(j_a' j_b' \lambda' | S_a' S_b')]$$

$$\times \left[\sum_{\kappa \mu_1 \mu_1''} \alpha^2(\kappa)(-1)^{\mu_1+\mu_1''} D^{\kappa}_{\mu_1 - \mu_1''}(S_a) D^{\kappa}_{-\mu_1 \mu_1''}(S_a') \right]$$

$$\times \left[\sum_{L_b \beta\mu} \alpha^2(L_b) D^{L_b}_{\beta,-\mu}(S_b) D^{L_b}_{\beta,-\mu}(S_b')^{\star} \right] \Bigg] \Bigg\} . \qquad (\text{I}.4\text{-}14)$$

The summations over κ, μ_1, and μ_1'' yield $(8\pi^2)\delta(S_a - S_a')$, while those over L_b, β, and μ yield $(8\pi^2)\delta(S_b - S_b')$. It is now possible to do the integrations over the six primed angles. After a convenient relabelling of indices,

$$\sigma' \begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k = \frac{\hbar^2 \pi^{3/2}}{4\mu k_B T} \Bigg\{ \Big[\sum_{\lambda} \alpha^2(\lambda) \Omega(0qq)^{-1/2} \Omega(0\ell\ell)^{-1/2} \alpha(\ell q)$$

$$\times \delta(\ell q t k | \ell' q' t' 0) \int d\gamma \, \gamma \, \mathcal{R}_{n\ell}(\gamma) \, \mathcal{R}_{n'\ell}(\gamma) \Big]$$

$$- 2\Omega(kqq')^{-1/2} \Omega(k\ell\ell')^{-1/2} (i)^{q-q'+\ell+\ell'} \alpha(\ell\ell') \left[\frac{\Gamma(n+1)\,\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\,\Gamma(n'+\ell'+3/2)} \right]^{1/2}$$

$$\times (8\pi^2)^{-2} \sum_{\substack{j_a' j_b' \\ \lambda\lambda'}} \Big[\alpha^2(\lambda\lambda') \alpha(j_a') (p_{j_a' j_b'}) ([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')})^{1/2}_{j_a'}$$

$$\sum_{\substack{\alpha\beta \\ \alpha'\beta'}} (i)^{\alpha+\beta+\alpha'+\beta'} \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & k & \ell' \\ 0 & \beta+\beta' & -\beta-\beta' \end{pmatrix} \begin{pmatrix} k & q & q' \\ -\beta-\beta' & \beta & \beta' \end{pmatrix}$$

(Equation continued on following page.)

$$\times\, R_{t'}^{(q')}(\epsilon_{j_a'}) \int d\gamma\, \gamma^{\ell+1}\, e^{-\gamma^2}\, L_{n'}^{\ell'+1/2}(\gamma^2) \iint dS_a dS_b\, S^{*}(j_a' j_b' \lambda' | S_a S_b)$$

$$\times\, D^{q'}_{\alpha'\beta'}(S_a)[E_a(q'j_a';-\alpha')I_a(q-\alpha)D^{q}_{\alpha\beta}(S_a)E^{*}_{ab}(\lambda\lambda'\xi';-\beta'-\beta)C^{*}_{ab}(\ell qnt)$$

$$\times\, S(j_a' j_b' \lambda | S_a S_b)]\Big]\Bigg\} \,. \qquad (I.4\text{-}15)$$

Further simplification of the above expression is difficult without restriction of one or more of the indices.

I.5 $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ in Terms of the Reduced Scattering Matrix

Equation (I.2-6) is an expression for $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ in terms of the kinetic theory cross section, $\sigma''(\ell n j_a j_b q|\ell' n' j_b' j_a' q')_k$, for nonvibrating diatomic molecules. HS-44 is an expression for $\sigma''(\ell n j_a j_b q|\ell' n' j_b' j_a' q')_k$ in terms of the relative velocity cross sections, $\sigma_1(\ell n|j_a j_b;qq'|\ell' n')_k$ and $\sigma_2(\ell n j_a j_b|L_a M_a L_b M_b;L_a' M_a' L_b' M_b'|\ell' n' j_b' j_a')_k$, which in turn are expressed in terms of quantities, F_λ, using HS-41 and HS-42:

$$\sigma_1(\ell n|j_a j_b;qq'|\ell' n')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{m}{8k_B T}\right)^{1/2} \Omega(k\ell\ell')^{-1/2} (-i)^{\ell+\ell'} \alpha(\ell\ell' k)$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} \int d\gamma \frac{\gamma^2}{\mu g} R_{n\ell}(\gamma) R_{n'\ell'}(\gamma)$$

$$\times \sum_{\lambda M_a} \alpha^2(\lambda) \begin{pmatrix} q & q' & k \\ M_a & -M_a & 0 \end{pmatrix} F_\lambda(j_a j_b;q M_a q' -M_a;j_a j_b) , \qquad (I.5-1)$$

and

$$\sigma_2(\ell n j_a j_b|L_a M_a L_b M_b;L_a' M_a' L_b' M_b'|\ell' n' j_b' j_a')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{m}{8k_B T}\right)^{1/2} \Omega(k\ell\ell')^{-1/2}$$

$$\times (-i)^{\ell+\ell'} \alpha(\ell\ell') \int d\gamma\gamma^2 \int dq'(g')^2 \frac{\sigma(E)}{qq'} R_{n\ell}(\gamma) R_{n'\ell'}(\gamma')$$

$$\times \sum_{\lambda\lambda'} \alpha^2(\lambda\lambda') \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & -M_a'-M_b' & M_a'+M_b'-M_a-M_b \end{pmatrix}$$

(Continued on following page.)

$$\times \begin{pmatrix} k & \ell & \ell' \\ M_a+M_b-M_a'-M_b' & 0 & M_a'+M_b'-M_a-M_b \end{pmatrix} F_\lambda(j_b'j_a';L_aM_aL_bM_b;j_aj_b)$$

$$\times F^*_{\lambda'}(j_b'j_a';L_a'M_a'L_b'M_b';j_aj_b) \;, \qquad \text{(I.5-2)}$$

yielding

$$\sigma''(\ell n j_a j_b q|\ell' n' j_b' j_a' q')_k = \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2} \Omega(k\ell\ell')^{-1/2}\, \Omega(kqq')^{-1/2}\, \alpha(\ell\ell')$$

$$\times \Bigg\{\Bigg[\delta(j_aj_b|j_b'j_a')(-i)^{-q-q'}\;(-1)^k\begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0\end{pmatrix} \int d\gamma\, \frac{\gamma^2}{\mu g}\, R_{n\ell}(\gamma)\, R_{n'\ell'}(\gamma)$$

$$\times \sum_{\lambda M_a} \alpha^2(\lambda)\begin{pmatrix} q & q' & k \\ M_a & -M_a & 0\end{pmatrix}\Big\{(-1)^{q+q'}\;(-i)^{\ell+\ell'}\;F_\lambda(j_aj_b;q\,M_a\,q'\,-M_a;j_aj_b)$$

$$+\;(-i)^{-\ell-\ell'}\;F^*_\lambda(j_aj_b;q\,M_a\,q'\,-M_a;j_aj_b)\Big\}\Bigg]$$

$$-\Bigg[(-1)^k\;(-i)^{\ell+\ell'-q+q'}\;(-1)^{j_a+j_b+j_a'+j_b'}\;\alpha(qq')\;\alpha^{-1}(j_b)\;\alpha^2(j_a')\;\alpha(j_b')$$

$$\times \sum_{\substack{L_aL_bM_aM_b\\ L_a'L_b'M_a'M_b'}}\;\sum_{\substack{\lambda\lambda' m\\ m'm''}} (-1)^{L_b+L_b'+M_a+M_b+M_a'+M_b'}\;\alpha(L_aL_b)\;\alpha(L_a'L_b')(-1)^{q+q'}$$

$$\times \alpha^2(\lambda\lambda')\begin{Bmatrix} j_b & L_b & j_a' \\ q' & j_a' & L_b'\end{Bmatrix}\begin{Bmatrix} q & L_a' & L_a \\ j_b' & j_a & j_a\end{Bmatrix}\begin{pmatrix} L_b' & L_b & q' \\ -M_b' & M_b & m''\end{pmatrix}\begin{pmatrix} q' & k & q \\ -m'' & m & m'\end{pmatrix}$$

$$\times \begin{pmatrix} q & L_a' & L_a \\ -m' & -M_a' & M_a\end{pmatrix}\begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & -M_a'-M_b' & -m\end{pmatrix}\begin{pmatrix} k & \ell & \ell' \\ M_a+M_b-M_a'-M_b' & 0 & -m\end{pmatrix}$$

(Equation continued on following page.)

$$\times \int d\gamma\gamma^2 \int dg'(g')^2 \frac{\delta(E)}{gg'} R_{n\ell}(\gamma)\, R_{n'\ell'}(\gamma')$$

$$\times F_\lambda(j_b' j_a'; L_a M_a L_b M_b; j_a j_b)\, F^*_{\lambda'}(j_b' j_a'; L_a' M_a' L_b' M_b'; j_a j_b) \Big] . \qquad \text{(I.5-3)}$$

The F_λ quantities are expressed in terms of the reduced scattering matrix using (I.3-5). This allows (I.5-[illegible]) to be rewritten upon explicit evaluation of certain sums:

$$\sigma''(\ell n j_a j_b q | \ell' n' j_b' j_a' q')_k = \frac{\hbar^{2}}{\mu}\left(\frac{\mu}{8 k_B T}\right)^{1/2} [illegible](k\ell\ell')^{-1/2}\, [illegible](kqq')^{-1/2}\, [illegible](\ell\ell')$$

$$\times \Bigg\{ \Big[2\delta(j_a j_b | j_b' j_a')\, \delta(\ell q q' k | \ell' 000) [illegible] \Big]$$

$$- \delta(j_a j_b | j_b' j_a')(-1)^{j_a' + j_b' + k}\, [illegible](j_a' j_b')\, [illegible](qq')\, (-i)^{[illegible]}$$

$$\times \begin{pmatrix} k & \ell & \ell' \\ 0 & 0 & 0 \end{pmatrix} \int d\gamma\, \frac{\gamma^2}{\mu g} R_{n\ell}(\gamma) R_{n'\ell'}(\gamma) \sum_{M_a} (-i)^{[illegible]} \begin{pmatrix} [illegible] & j_b' & q \\ [illegible] & [illegible] & [illegible] \end{pmatrix}$$

$$\times \begin{pmatrix} j_a' & j_a' & q' \\ 0 & \mu & -\mu \end{pmatrix} [illegible](\lambda) \begin{pmatrix} q & q' & k \\ M_a & -M_a & 0 \end{pmatrix} (8\pi^2)^{-2}$$

$$\times \iint dS_a dS_b \Big[S(j_b' j_a' \lambda | S_a S_b) D^q_{\nu M_a}(S_a) D^{q'}_{\mu - M_a}(S_b)$$

$$+ (-1)^{q + q' + [illegible]} S^*(j_b' j_a' \lambda | S_a S_b) D^{q}_{[illegible] M_a}(S_a)^* D^{q'}_{[illegible] -M_a}(S_b)^* \Big] \Bigg\}$$

(Equation continued on following page.)

$$
- \frac{\hbar^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2} \Omega(k\ell\ell')^{-1/2}\ \Omega(kqq')^{-1/2}\ \alpha(\ell\ell')
$$

$$
\times \Bigg\{ \left[\delta(j_aj_b|j_b'j_a')\delta(\ell qq'k|\ell'000)\alpha^{-1}(\ell) \sum_{\lambda} \alpha^2(\lambda) \int d\gamma\ \frac{\gamma^2}{\mu g} R_{n\ell}(\gamma)R_{n'\ell}(\gamma) \right]
$$

$$
- \delta(j_aj_b|j_b'j_a')(-1)^{j_a'+j_b'+k}\alpha(j_a'j_b')\alpha(qq')(-i)^{q+q'+\ell+\ell'}
$$

$$
\times \int d\gamma\ \frac{\gamma^2}{\mu g} R_{n\ell}(\gamma)R_{n'\ell'}(\gamma) \sum_{\substack{\lambda\lambda' M_a \\ \nu\mu M_b}} \alpha^2(\lambda') \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & 0 & -M_a-M_b \end{pmatrix}
$$

$$
\times (-i)^{\nu+\mu+M_a+M_b} \begin{pmatrix} j_b' & j_b' & q \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_a' & j_a' & q' \\ 0 & \mu & -\mu \end{pmatrix} \alpha^2(\lambda) \begin{pmatrix} q & q' & k \\ M_a & M_b & -M_a-M_b \end{pmatrix}
$$

$$
\times \begin{pmatrix} k & \ell & \ell' \\ M_a+M_b & 0 & -M_a-M_b \end{pmatrix} (8\pi^2)^{-2} \iint dS_a dS_b [S(j_b'j_a'\lambda|S_aS_b)D^q_{\nu M_a}(S_a)D^{q'}_{\mu M_b}(S_b)
$$

$$
+ (-1)^{q+q'+\lambda+\lambda'+\nu+\mu} S^*(j_b'j_a'\lambda|S_aS_b)\ D^q_{\nu M_a}(S_a)^*\ D^{q'}_{\mu M_b}(S_b)^*]
$$

$$
+ (-i)^{q-q'+\ell+\ell'} (-1)^{k+j_a+j_b+j_a'+j_b'}\ \alpha^2(j_aj_a')\ \alpha(j_bj_b')\ \alpha(qq')
$$

$$
\times \sum_{\substack{L_aL_bM_aM_b \\ L_a'L_b'M_a'M_b' \\ \nu\mu\nu'\mu'}} \sum_{\lambda\lambda'} \left[(-i)^{\nu+\mu-\nu'-\mu'} (-i)^{M_a'+M_b'-M_a-M_b} (-1)^{L_b+L_b'} \right.
$$

$$
\times \alpha^2(\lambda\lambda')\alpha(L_aL_b)\alpha(L_a'L_b') \begin{Bmatrix} j_b & L_b & j_a' \\ q' & j_a' & L_b' \end{Bmatrix} \begin{Bmatrix} q & L_a' & L_a \\ j_b' & j_a & j_a \end{Bmatrix} \begin{pmatrix} L_b' & L_b & q' \\ -M_b' & M_b & M_b'-M_b \end{pmatrix}
$$

(Equation continued on following page.)

$$\times \begin{pmatrix} q' & k & q \\ M_b-M_b' & M_a'+M_b'-M_a-M_b & M_a-M_a' \end{pmatrix} \begin{pmatrix} q & L_a' & L_a \\ M_a'-M_a & -M_a' & M_a \end{pmatrix} \cdots$$

$$\times \begin{pmatrix} \lambda & \lambda' & \lambda' \\ M_a+M_b & -M_a'-M_b' & M_a'+M_b'-M_a-M_b \end{pmatrix} \begin{pmatrix} k & & \\ M_a+M_b-M_a'-M_b' & 0 & M_a'+M_b'-M_a-M_b \end{pmatrix}$$

$$\times \begin{pmatrix} j_a & j_b' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_a' & L_b \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} j_a & j_b' & L_a' \\ 0 & \nu' & -\nu' \end{pmatrix} \begin{pmatrix} j_b & j_a' & L_b' \\ 0 & \mu' & -\mu' \end{pmatrix}$$

$$\times (8\pi^2)^{-4} \int d\gamma\, \gamma^2 \int dg'(g')^2 \frac{\partial(E)}{\partial g'} R_{n\ell}(\gamma)\, R_{n'\ell'}(\gamma')$$

$$\times \iiiint dS_a dS_b dS_a' dS_b'\; S(j_b'j_a'\lambda'|S_a S_b)\; S^*(j_b'j_a'\lambda'|S_a'S_b')$$

$$\times D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)\, D^{L_a'}_{\nu' M_a'}(S_a')^*\, D^{L_b'}_{\mu' M_b'}(S_b')^* \Big]\Big\} \,. \qquad \text{(I.5-4)}$$

The sum over λ' gives[8,9] $\delta(M_a+M_b|0) = \delta(M_a|-M_b)$, which causes the terms in (I.5-4) that are linear in S to vanish. Insertion of the remaining terms of (I.5-4) in (I.2-6) yields a useful first expression for $\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k$ in terms of the reduced scattering matrix:

$$\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k = \frac{5^2\pi}{\mu}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2} \Big\{ \Big[\sum_{j_a'j_b'} (\rho_{j_a'j_b'})([J]^{(q)} \odot^q [J]^{(q)})^{1/2}_{j_b'}$$

$$\times ([J]^{(q')} \odot^{q'} [J]^{(q')})^{1/2}_{j_a'}\, R_t^{(q)}(\varepsilon_{j_b'})\, R_{t'}^{(q')}(\varepsilon_{j_a'})$$

$$\times \alpha^2(\lambda)\, \Omega(0::)^{-1/2}\, (\ldots)\, (\ldots qq'k \ldots 000) \int d\gamma \frac{\gamma^2}{\mu q} \ldots (\gamma)\, R \ldots (\gamma)$$

(Equation continued on following page.)

$$
\begin{aligned}
&- \Omega(kqq')^{-1/2}\, \Omega(k\ell\ell')^{-1/2}\, (-i)^{q-q'+\ell+\ell'}\, \alpha(\ell\ell') \\
&\times \Bigg[\sum_{\substack{j_a j_b \\ j'_a j'_b}} \alpha^2(j_a j'_a)\alpha^2(j_b j'_b)(p_{j_a j_b j'_a j'_b})^{1/2} \left([\underline{J}]^{(q)} \odot^{q} [\underline{J}]^{(q)}\right)^{1/2}_{j_a} \\
&\times \left([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')}\right)^{1/2}_{j'_a} R_t^{(q)}(\varepsilon_{j_a})\, R_{t'}^{(q')}(\varepsilon_{j'_a})\, (-1)^{k+j_a+j_b+j'_a+j'_b} \\
&\times \sum_{\substack{L_a L_b M_a M_b \\ L'_a L'_b M'_a M'_b}} \sum_{\substack{\nu\mu\nu'\mu' \\ \lambda\lambda'}} (-i)^{\nu+\mu-\nu'-\mu'}\, (-i)^{M'_a+M'_b-M_a-M_b}\, (-1)^{L_b+L'_b} \\
&\times \alpha^2(\lambda\lambda')\, \alpha^2(L_a L_b)\, \alpha^2(L'_a L'_b) \begin{Bmatrix} j_b & L_b & j'_a \\ q' & j'_a & L'_b \end{Bmatrix} \begin{Bmatrix} q & L'_a & L_a \\ j'_b & j_a & j_a \end{Bmatrix} \\
&\times \begin{pmatrix} L'_b & L_b & q' \\ -M'_b & M_b & M'_b-M_b \end{pmatrix} \begin{pmatrix} q' & k & q \\ M_b-M'_b & M'_a+M'_b-M_a-M_b & M_a-M'_a \end{pmatrix} \begin{pmatrix} q & L'_a & L_a \\ M'_a-M_a & -M'_a & M_a \end{pmatrix} \\
&\times \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ M_a+M_b & -M'_a-M'_b & M'_a+M'_b-M_a-M_b \end{pmatrix} \\
&\times \begin{pmatrix} k & \ell & \ell' \\ M_a+M_b-M'_a-M'_b & 0 & M'_a+M'_b-M_a-M_b \end{pmatrix} \begin{pmatrix} j_a & j'_b & L_a \\ 0 & \nu & -\nu \end{pmatrix} \\
&\times \begin{pmatrix} j_b & j'_a & L_b \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} j_a & j'_b & L'_a \\ 0 & \nu' & -\nu' \end{pmatrix} \begin{pmatrix} j_b & j'_a & L'_b \\ 0 & \mu' & -\mu' \end{pmatrix} \int d\gamma\,\gamma^2 \int dg'\,(g')^2\, \frac{\delta(E)}{gg'} \\
&\times R_{n\ell}(\gamma) R_{n'\ell'}(\gamma')(8\pi^2)^{-4} \iiiint dS_a\, dS_b\, dS'_a\, dS'_b\; S(j'_b j'_a \lambda | S_a S_b) \\
&\times S^*(j'_b j'_a \lambda' | S'_a S'_b) D^{L_a}_{\cdot M_a}(S_a) D^{L_b}_{\cdot M_b}(S_b) D^{L'_a}_{\cdot M'_a}(S'_a)^* D^{L'_b}_{\cdot M'_b}(S'_b)^* \Bigg] \Bigg\} . \qquad \text{(I.5-5)}
\end{aligned}
$$

As in (I.3-16), the integration over the energy delta-function can be done. Switching the indices, j_a' and j_b',

$$\sigma''\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\Bigg\{\Bigg[\sum_{j_a' j_b' \lambda} \alpha^2(\lambda)(\rho_{j_a' j_b'})\Omega(0\ell\ell)^{-1/2}\,\iota(\ell\ell)$$

$$\times\ \delta(\ell qq'k|\lambda'000)\, R_t^{(0)}(\varepsilon_{j_a'})R_{t'}^{(0)}(\varepsilon_{j_b'}) \int d\gamma\gamma\, R_{n\ell}(\gamma)R_{n'\ell'}(\gamma)$$

$$-\ 2\Omega(kqq')^{-1/2}\,\Omega(k\ell\ell')^{-1/2}\,(-i)^{q-q'+\ell+\ell'}\,\iota(\ell\ell')$$

$$\times \Bigg[\sum_{\substack{j_a j_b\\ j_a' j_b'}} \alpha^3(j_a)\alpha^2(j_b)\alpha(j_a')(\rho_{j_a' j_b'})\left([\underline{J}]^{(q)}\odot^q[\underline{J}]^{(q)}\right)^{1/2}_{j_a}$$

$$\times \left([\underline{J}]^{(q')}\odot^{q'}[\underline{J}]^{(q')}\right)^{1/2}_{j_b'} R_{t'}^{(q')}(\varepsilon_{j_b'})(-1)^{k+j_a+j_b+j_a'+j_b'}$$

$$\times \sum_{\substack{L_aL_bM_aM_b\\ L_a'L_b'M_a'M_b'}}\ \sum_{\substack{\nu'\mu'\\ \lambda\lambda'}} (-i)^{M_a'+M_b'-M_a-M_b-\nu'-\mu'}\ (-1)^{L_b+L_b'}\,\iota(\lambda\lambda')\,\alpha^2(L_aL_b)$$

$$\times\ \alpha^2(L_a'L_b')\begin{Bmatrix} j_b & L_b & j_b'\\ q' & j_b' & L_b'\end{Bmatrix}\begin{Bmatrix} q & L_a' & L_a\\ j_a' & j_a & j_a\end{Bmatrix}\begin{pmatrix} L_b' & L_b & q\\ -M_b' & M_b & M_b'-M_b\end{pmatrix}$$

$$\times \begin{pmatrix} q' & k & q\\ M_b-M_b' & M_a'+M_b'-M_a-M_b & M_a-M_a'\end{pmatrix}\begin{pmatrix} q & L_a' & L_a\\ M_a'-M_a & -M_a' & M_a\end{pmatrix}\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}$$

$$\times \begin{pmatrix}\lambda & \lambda' & \ell'\\ M_a+M_b & -M_a'-M_b' & M_a'+M_b'-M_a-M_b\end{pmatrix}\begin{pmatrix} k & \ell & \ell'\\ M_a+M_b-M_a'-M_b' & 0 & M_a'+M_b'-M_a-M_b\end{pmatrix}$$

(Equation continued on following page.)

$$\times \begin{pmatrix} j_a & j'_a & L'_a \\ 0 & \nu' & -\nu' \end{pmatrix} \begin{pmatrix} j_b & j'_b & L'_b \\ 0 & \mu' & -\mu' \end{pmatrix} \left[\frac{\Gamma(n+1)\,\Gamma(n'+1)}{\Gamma(n+\ell+\tfrac{1}{2})\,\Gamma(n'+\ell'+\tfrac{1}{2})} \right]^{\frac{1}{2}}$$

$$\times (8\pi^2)^{-4} \int d\gamma\, \gamma^{\ell+1}\, e^{-\gamma^2}\, L_{n'}^{\ell'+\frac{1}{2}}(\gamma^2) \iiiint dS_a\, dS_b\, dS'_a\, dS'_b$$

$$\times S(j'_a j'_b \lambda | S_a S_b)\, S^{*}(j'_a j'_b \lambda' | S'_a S'_b)\, D^{L'_a}_{\nu' M'_a}(S'_a)^{*}\, D^{L'_b}_{\mu' M'_b}(S'_b)^{*}\, P_t^{(q)}(\varepsilon_{j_a})$$

$$\times [\gamma^2 + \varepsilon_{j'_a} + \varepsilon_{j'_b} - \varepsilon_{j_a} - \varepsilon_{j_b}]^{\ell/2}\, L_n^{\ell+\frac{1}{2}}(\gamma^2 + \varepsilon_{j'_a} + \varepsilon_{j'_b} - \varepsilon_{j_a} - \varepsilon_{j_b})$$

$$\times \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j'_a & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j'_b & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b) \Bigg] \Bigg\} \,. \qquad (I.5\text{-}6)$$

Further simplification of $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ requires the introduction of operators analogous to those introduced in section I.4. This reduction of the $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ collision integrals is accomplished in the next section.

I.6 Reduction of the $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ Collision Integrals

In this section, equation (I.5-...) is reduced from a summation over nineteen indices and an integration over twelve angles to an eight-fold summation and a six-fold angle integration. The reduction closely parallels that of $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ in section I.4, and therefore will be discussed in somewhat less detail than that of $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$.

It is shown in section I.4 that

$$\iiiint dS_a dS_b dS_a' dS_b' \; S(j_a'j_b'\lambda|S_aS_b)\, S^*(j_a'j_b'\lambda'|S_a'S_b')\, D^{L_a'}_{\nu'M_a'}(S_a')^* \, D^{L_b'}_{\mu'M_b'}(S_b')^*$$

$$\times \Big\{ R_t^{(q)}(\varepsilon_{j_a})[\gamma^2 + \varepsilon_{j_a'} + \varepsilon_{j_b'} - \varepsilon_{j_a} - \varepsilon_{j_b}]^{\ell/2}$$

$$\times \; L_n^{\ell+\frac{1}{2}}(\gamma^2 + \varepsilon_{j_a'} + \varepsilon_{j_b'} - \varepsilon_{j_a} - \varepsilon_{j_b})\Big\}$$

$$\times \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)$$

$$= \iiiint dS_a dS_b dS_a' dS_b' \; S(j_a'j_b'\lambda|S_aS_b)\, S^*(j_a'j_b'\lambda'|S_a'S_b')\, D^{L_a'}_{\nu'M_a'}(S_a')^* \, D^{L_b'}_{\mu'M_b'}(S_b')^*$$

$$\times\; C_{ab}(\ell qnt) \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j_a' & L_a \\ 0 & \nu & -\nu \end{pmatrix} \begin{pmatrix} j_b & j_b' & L_b \\ 0 & \mu & -\mu \end{pmatrix} D^{L_a}_{\nu M_a}(S_a)\, D^{L_b}_{\mu M_b}(S_b)$$

(I.6-1a)

$$= \sum_{\nu\mu} (-i)^{\nu+\mu} \begin{pmatrix} j_a & j'_a & L_a \\ 0 & \nu & -\nu \end{pmatrix} \ldots \, dS'_a \, dS'_b$$

$$\times [C^{\star}_{ab}(\varepsilon qnt) \, S(j'_a j'_b \ldots$$

$$\times S^{\star}(j'_a j'_b \lambda' | S'_a S'_b) \, D^{L'_a}_{\ldots} \ldots \quad (1.6\text{-}1b)$$

Once the above is utilized [illegible]

evaluated:[8]

$$\sum_{j_b} (-1)^{j_b} \ldots (j_b) \begin{Bmatrix} j_b & L_b & \ldots \\ q' & j'_b & \ldots \end{Bmatrix} \ldots$$

$$= (-1)^{\ldots} \begin{pmatrix} j'_b & j'_a & \ldots \\ -\mu' & \ldots \end{pmatrix} \ldots \quad (1.6\text{-}2)$$

Making use of the relation

$$\begin{Bmatrix} q & L'_a & L_a \\ j'_a & j_a & j_a \end{Bmatrix} \begin{pmatrix} j_a & j'_a & L_a \\ 0 & \nu & -\nu \end{pmatrix} \ldots$$

$$\ldots \begin{pmatrix} j_a & q & L_a \\ 0 & \ldots & -\nu \end{pmatrix} \begin{pmatrix} \ldots & L_a \\ \ldots \end{pmatrix} \ldots \quad (1.6\text{-}3)$$

and relabelling indices yields

$$\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k = \frac{\hbar}{4\pi k_B T} \text{[illegible]} \; \alpha(\ell)$$

$$\times\ \delta(\ell q q' k \ell' 000) R_t^{(0)} \text{[illegible]} \Big]$$

$$-\ 2\Omega(kqq')^{-1/2}\ \Omega(k\ell\ell') \text{[illegible]}$$

$$\times \Bigg[\sum_{\substack{\lambda\lambda' j_a' j_b' j_a \\ L_a L_b L_a' L_b'}} \text{[illegible]} (j_a) \text{[illegible]} \Big)^{1/2}_{j_a}$$

$$\times\ \left([J]^{(q')} \mathcal{J}' [J]^{(q')} \right)^{1/2}_{j_b'} (-1) \text{[illegible]} (L_a L_b) \text{[illegible]} (L_a' L_b')$$

$$\times \sum_{\substack{\alpha\beta\nu M_a \delta \\ \alpha'\beta'\nu' M_a'}} (-i)^{-\alpha-\beta-\text{[illegible]}} \text{[illegible]} \begin{pmatrix} \text{[illegible]} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \lambda' & \ell' \\ -\nu & \nu' & \nu-\nu' \end{pmatrix}$$

$$\times \begin{pmatrix} j_a & j_a' & L_a' \\ 0 & \alpha' & -\alpha' \end{pmatrix} \begin{pmatrix} j_b' & j_b & q' \\ -\beta' & \beta & \text{[illegible]} \end{pmatrix} \begin{pmatrix} q' & L_b & L_b' \\ \text{[illegible]} \end{pmatrix} \begin{pmatrix} \ell & k & \ell' \\ 0 & \nu'-\nu & \nu-\nu' \end{pmatrix}$$

$$\times \begin{pmatrix} k & q' & q \\ \nu'-\nu & \nu-\nu'+M_a-M_a' & M_a'-M_a \end{pmatrix} \begin{pmatrix} q & L_a & L_a' \\ M_a'-M_a & M_a & -M_a' \end{pmatrix}$$

$$\times \begin{pmatrix} q' & L_b & L_b' \\ \nu-\nu'+M_a-M_a' & -\nu-M_a & \nu'+M_a' \end{pmatrix} \begin{pmatrix} j_a & q & j_a \\ 0 & \text{[illegible]} & \text{[illegible]} \end{pmatrix} \begin{pmatrix} L_a' & j_a' & j_a \\ \text{[illegible]} & & \delta \end{pmatrix} \begin{pmatrix} L_a' & q & L_a \\ \delta+\alpha & -\delta & -\alpha \end{pmatrix}$$

$$\times\ (8\pi^2)^{-4} \left[\frac{\Gamma(n+1)\,\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\,\Gamma(n'+\ell'+3/2)} \right]^{1/2} R_{t'}^{(q')}(\text{[illegible]}_{j_b'}) \int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}$$

(Equation continued on following page.)

$$\times\, L_{n'}^{\ell'+1/2}(\gamma^2) \iiiint dS_a dS_b dS_a' dS_b' [C_{ab}^{*}(\ell qnt)\; S(j_a'j_b'\lambda|S_aS_b)]$$

$$\times\, D_{\alpha M_a}^{L_a}(S_a) D_{\beta,-\nu-M_a}^{L_b}(S_b)\; S^{*}(j_a'j_b'\lambda'|S_a'S_b') D_{\alpha' M_a'}^{L_a'}(S_a')^{*} D_{\beta',-\nu'-M_a'}^{L_b'}(S_b')^{*}\Big]\Big\}. \tag{I.6-4}$$

At this point it is again convenient to introduce the $E_{ab}(\lambda\lambda'\ell';\nu-\nu')$ and $E_{b'}(q'j_b';\beta-\beta')$ operators of section I.4. Now, the L_a and L_b' summations can be carried out as in (I.4-8a) and (I.4-8b). Making use of the fact that these operators are hermitian and relabelling indices allows (I.6-4) to be written

$$\sigma''\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\left\{\left[\sum_{j_a'j_b'\lambda} \alpha^2(\lambda)(p_{j_a'j_b'})\Omega(0\ell\ell)^{-1/2}\,\alpha(\ell)\right.\right.$$

$$\left.\times\,\delta(\ell qq'k|\ell'000)R_t^{(0)}(\varepsilon_{j_a'})R_{t'}^{(0)}(\varepsilon_{j_b'}) \int d\gamma\gamma\; R_{n\ell}(\gamma)\; R_{n'\ell}(\gamma)\right]$$

$$-\,2\Omega(kqq')^{-1/2}\;\Omega(k\ell\ell')^{-1/2}\;(i)^{q+q'+\ell+\ell'}\;\alpha(\ell\ell')\left[\frac{\Gamma(n+1)\;\Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2}$$

$$\times\,(8\pi^2)^{-4}\left[\sum_{\substack{\lambda\lambda' j_a'j_b'\\ j_aL_a'L_b}} \alpha^3(j_a)\;\alpha(j_b')\;(p_{j_a'j_b'})([\underline{J}]^{(q)}\odot^{\beta}[\underline{J}]^{(q)})_{j_a}^{1/2}\right.$$

$$\times\,([\underline{J}]^{(q')}\odot^{\beta'}[\underline{J}]^{(q')})_{j_b'}^{1/2}\;(-1)^{L_a'+j_a}\;\alpha^2(\lambda\lambda')\;\alpha^2(L_a'L_b)$$

$$\times \sum_{\substack{\alpha\alpha'\beta M_a'M_b\\ \nu\mu\nu'\mu'}} (-i)^{\alpha-\alpha'+\mu+\mu'-\nu-\nu'}\;(-1)^{\beta+M_b}\begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & k & \ell'\\ 0 & \nu+\nu' & -\nu-\nu'\end{pmatrix}$$

(Equation continued on following page.)

$$\times \begin{pmatrix} k & q & q' \\ -\nu-\nu' & \nu & \nu' \end{pmatrix} \begin{pmatrix} j_a & j_a' & L_a' \\ 0 & \alpha' & -\alpha' \end{pmatrix} \begin{pmatrix} j_a & q & j_a \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} L_a' & j_a' & j_a \\ -\alpha & \alpha-\mu & \mu \end{pmatrix} R_{+}^{(q')}(\text{[illegible]}\, j_b' \text{[illegible]})$$

$$\times \int d\gamma\, \gamma^{\ell+1}\, e^{-\gamma^2}\, L_{n'}^{\ell'+1/2}(\gamma^2) \iint dS_a dS_b [C_{ab}^{*}(\lambda\lambda' \text{[illegible]}) C_{ab}^{*}(\text{[illegible]})$$

$$\times S(j_a' j_b' \lambda | S_a S_b)] D_{\alpha M_a'}^{L_a'}(S_a) D_{-\mu\nu}^{q}(S_a) D_{\beta M_b}^{L_b}(S_b)$$

$$\times \iint dS_a' dS_b' [E_{b'}^{*}(q' j_b'; \mu') S^{*}(j_a' j_b' \lambda' | S_a' S_b')]$$

$$\times D_{\alpha' M_a'}^{L_a'}(S_a')^{*}\, D_{-\beta-M_b}^{L_b}(S_b')\, D_{\mu'\nu'}^{q'}(S_b') \Bigg]\Bigg\} . \qquad (I.6-5)$$

Next, the sum over j_a is treated:

$$\sum_{j_a} \alpha^3(j_a)\left([\underline{J}]^{(q)} \odot^{q} [\underline{J}]^{(q)}\right)^{1/2}_{j_a} \begin{pmatrix} j_a & j_a' & L_a' \\ 0 & \alpha' & -\alpha' \end{pmatrix} \begin{pmatrix} j_a & q & j_a \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} L_a' & j_a' & j_a \\ -\alpha & \alpha-\mu & \mu \end{pmatrix}$$

$$\equiv (-1)^{j_a'+L_a'}\, I(q\mu; L_a' j_a' \alpha, -\alpha') , \qquad (I.6-6)$$

making the introduction of the $I_{a'}(q\mu)$ operators of section I.4 possible. This allows the sums over L_a', M_a', α, L_b, M_b, and β to be evaluated:

$$\sum_{\substack{L_a'M_a'\alpha \\ L_bM_b\beta}} \alpha^2(L_a'L_b)(-1)^{\beta+M_b'} D^{L_a'}_{\alpha M_a'}(S_a) D^{L_b}_{\beta M_b}(S_b) D^{L_a'}_{\alpha M_a'}(S_a')^* \, D^{L_b}_{-\beta-M_b}(S_b')$$

$$= \left[\sum_{L_a'M_a'\alpha} \alpha^2(L_a') D^{L_a'}_{\alpha M_a'}(S_a) D^{L_a'}_{\alpha M_a'}(S_a')^*\right]\left[\sum_{L_bM_b\beta} \alpha^2(L_b) D^{L_b}_{\beta M_b}(S_b) D^{L_b}_{\beta M_b}(S_b')^*\right]$$

$$= (8\pi^2)^2 \, \delta(S_a - S_a') \, \delta(S_b - S_b') \ . \qquad (I.6\text{-}7)$$

The integrations over the angles S_a' and S_b' can now be performed, yielding

$$\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k = \frac{\hbar^2 \pi^{3/2}}{4\mu k_B T} \Bigg\{ \Bigg[\sum_{j_a'j_b'\lambda} \alpha^2(\lambda)(p_{j_a'j_b'}) \, \Omega(0\lambda\lambda)^{-1/2} \, \alpha(\lambda)$$

$$\times \, \delta(\ell q q' k | \ell' 000) R_t^{(0)}(\varepsilon_{j_a'}) R_{t'}^{(0)}(\varepsilon_{j_b'}) \int d\gamma \gamma \, R_{n\ell}(\gamma) \, R_{n'\ell}(\gamma) \Bigg]$$

$$- \, 2\Omega(kqq')^{-1/2} \, \Omega(k\ell\ell')^{-1/2} \, (i)^{q+q'+\ell+\ell'} \, \alpha(\ell\ell') \left[\frac{\Gamma(n+1) \, \Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2}$$

$$\times \, (8\pi^2)^{-2} \Bigg[\sum_{\substack{j_a'j_b' \\ \lambda\lambda'}} \alpha(j_b')(p_{j_a'j_b'}) \, \alpha^2(\lambda\lambda') \sum_{\nu\mu\nu'\mu'} (-i)^{\mu+\mu'-\nu-\nu'}$$

$$\times \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & k & \ell' \\ 0 & \nu+\nu' & -\nu-\nu' \end{pmatrix} \begin{pmatrix} k & q & q' \\ -\nu-\nu' & \nu & \nu' \end{pmatrix} \left([\underline{J}]^{(q')} \odot^{q'} [\underline{J}]^{(q')} \right)^{1/2}_{j_b'}$$

$$\times \, R_{t'}^{(q')}(\varepsilon_{j_b'}) \int d\gamma \, \gamma^{\ell+1} \, e^{-\gamma^2} \, L_{n'}^{\ell'+1/2}(\gamma^2)$$

(Equation continued on following page.)

$$\times \iint dS_a dS_b [E^*_{ab}(\lambda\lambda'\ell';-\nu-\nu')C^*_{ab}(\ell qnt)S(j_a'j_b'\lambda|S_aS_b)]D^q_{-\mu\nu}(S_a)D^{q'}_{\mu'\nu'}(S_b)$$

$$\left.\times [I_a^{\dagger *}(q\mu)E^*_b(q'j_b';\mu')S^*(j_a'j_b'\lambda'|S_aS_b)]\Bigg]\right\} . \qquad (I.6\text{-}8)$$

A final relabelling of indices produces an expression for $\sigma''\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k$ that is closely analogous to that of $\sigma'\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k$:

$$\sigma''\begin{pmatrix}\ell & q & n & t\\ \ell' & q' & n' & t'\end{pmatrix}_k = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\left\{\left[\sum_{j_a'j_b'\lambda} \alpha^2(\lambda)(p_{j_a'j_b'})\Omega(0\ell\ell)^{-1/2}\,\iota(\ell)\right.\right.$$

$$\left.\times\, \delta(\ell qq'k|\ell'000)R_t^{(0)}(\varepsilon_{j_a'})R_{t'}^{(0)}(\varepsilon_{j_b'}) \int d\gamma\gamma\, R_{n\ell}(\gamma)\, R_{n'\ell}(\gamma)\right]$$

$$- 2\Omega(kqq')^{-1/2}\,\Omega(k\ell\ell')^{-1/2}\,(i)^{q+q'+\ell+\ell'}\,\alpha(\ell\ell')\left[\frac{\Gamma(n+1)\,\Gamma(n'+1)}{\Gamma(n+\ell+1/2)\Gamma(n'+\ell'+1/2)}\right]^{1/2}$$

$$\times (8\pi^2)^{-2}\left[\sum_{\substack{j_a'j_b'\\ \lambda\lambda'}} \alpha^2(\lambda\lambda')\alpha(j_b')(p_{j_a'j_b'}) \sum_{\substack{\alpha\beta\\ \alpha'\beta'}} (i)^{\alpha+\beta-\alpha'+\beta'}\right.$$

$$\times \begin{pmatrix}\lambda & \lambda' & \ell'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell & k & \ell'\\ 0 & \beta+\beta' & -\beta-\beta'\end{pmatrix}\begin{pmatrix}k & q & q'\\ -\beta-\beta' & \beta & \beta'\end{pmatrix}$$

$$\times \left([\underline{J}]^{(q')}\odot^{q'}[\underline{J}]^{(q')}\right)^{1/2}_{j_b'} R_{t'}^{(q')}(\varepsilon_{j_b'}) \int d\gamma\, \gamma^{\ell+1}\, e^{-\gamma^2}\, L_{n'}^{\ell'+1/2}(\gamma^2)$$

$$\times \iint dS_a dS_b\, S^*(j_a'j_b'\lambda'|S_aS_b)[E_b(q'j_b';\alpha')D^{q'}_{\alpha'\beta'}(S_b)I_a(q-\alpha)D^q_{\alpha\beta}(S_a)$$

$$\left.\left.\times\, E^*_{ab}(\lambda\lambda'\ell';-\beta-\beta')C^*_{ab}(\ell qnt)S(j_a'j_b'\lambda|S_aS_b)]\Bigg]\right\} . \qquad (I.6\text{-}9)$$

As with equation (I.4-15), further simplification of (I.6-9) is difficult without restriction of one or more of the indices. Explicit evaluation of special cases of the $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ yield interesting relationships among the $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}(a)$. Some of these are examined in the next section.

I.7 Relations Among the $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$

Chen, Moraal, and Snider[4] have examined the $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}_k$ collision integrals in the special case in which one of the $\underset{\sim}{B}_{pqst}$ basis operators is purely translational, i.e., $q' = t' = 0$. These exhibit interesting relations due to the nature of the $\sigma'(\ell n j_a j_b q|\ell' n' j_a' j_b' 0)_k$ and $\sigma''(\ell n j_a j_b q|\ell' n' j_b' j_a' 0)_k$ cross sections. The $\sigma\begin{pmatrix} p & q & s & t \\ p' & 0 & s' & 0 \end{pmatrix}^{(a)}$ exhibit similar relations because the $\sigma'\begin{pmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{pmatrix}_k$ and $\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{pmatrix}_k$ collision integrals are themselves closely related to the cross sections.[12] In this section, the $\sigma'\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k$ and $\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}_k$ collision integrals are examined in the $q' = t' = 0$ special case and relations among the $\sigma\begin{pmatrix} p & q & s & t \\ p' & 0 & s' & 0 \end{pmatrix}^{(a)}$ scalars analogous to those of Chen, Moraal, and Snider are obtained.

If the restriction is made that $q' = t' = 0$, equation (I.6-9) can be simplified using the following:

$$E_b(0j_b';0) = \alpha^{-1}(j_b') , \tag{I.7-1}$$

$$D^0_{\alpha'\beta'}(S_b) = \delta(\alpha'\beta'|00) , \tag{I.7-2a}$$

$$\begin{pmatrix} k & q & 0 \\ -\beta & \beta & 0 \end{pmatrix} = (-1)^{q-\beta}\, \alpha^{-1}(q)\, \delta(q|k) , \tag{I.7-2b}$$

$$([\underset{\sim}{J}]^{(0)}\odot^{(0)}[\underset{\sim}{J}]^{(0)})^{1/2}_{j_b'} = 1 \; , \tag{I.7-3a}$$

$$R_0^{(0)}(\varepsilon_{j_b'}) = 1 \; , \tag{I.7-3b}$$

and

$$\sum_{j_a' j_b'} (p_{j_a' j_b'}) R_t^{(0)}(\varepsilon_{j_a'}) R_0^{(0)}(\varepsilon_{j_b'}) = \delta(t|0) \; . \tag{I.7-3c}$$

Thus (I.6-9) becomes

$$\begin{aligned}
\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{pmatrix}_k = \frac{\hbar^2 \pi^{3/2}}{4\mu k_B T} \Bigg\{ & \Bigg[\sum_\lambda \alpha^2(\lambda)\Omega(0\ell\ell)^{-1/2} \alpha(\ell)\ \delta(\ell q t k|\ell' 000) \\
& \times \int d\gamma\gamma\ R_{n\ell}(\gamma)\ R_{n'\ell}(\gamma) \Bigg] \\
& - 2\Omega(qq0)^{-1/2}\ \Omega(q\ell\ell')^{-1/2}\ (-i)^{q-\ell-\ell'}\ \alpha^{-1}(q)\ \alpha(\ell\ell')\ \delta(k|q) \\
& \times \left[\frac{\Gamma(n+1)}{\Gamma(n+\ell+\frac{3}{2})} \frac{\Gamma(n'+1)}{\Gamma(n'+\ell'+\frac{3}{2})} \right]^{1/2} (8\pi^2)^{-2} \Bigg[\sum_{\substack{j_a' j_b' \\ \lambda\lambda'}} \alpha^2(\lambda\lambda')\ (p_{j_a' j_b'}) \\
& \times \sum_{\alpha\beta} (i)^{\alpha-\beta} \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & q & \ell' \\ 0 & \beta & -\beta \end{pmatrix} \int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n'}^{\ell'+1/2}(\gamma^2) \\
& \times \iint dS_a dS_b\ S^*(j_a' j_b' \lambda' | S_a S_b)\ I_a(q-\alpha) D^q_{\alpha\beta}(S_a) \\
& \times E^*_{ab}(\lambda\lambda'\ell';-\beta) C^*_{ab}(\ell q n t)\ S(j_a' j_b' \lambda | S_a S_b) \Bigg] \Bigg\} \; .
\end{aligned} \tag{I.7-4}$$

A similar treatment of equation (I.4-15) yields the important result:

$$\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell'0 & & n'0 \end{Bmatrix}_k = \sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell'0 & & n'0 \end{Bmatrix}_k = \delta(k|q)\ \sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell'0 & & n'0 \end{Bmatrix}_q \ . \qquad \text{(I.7-5)}$$

Equation (I.7-5) can now be used to obtain an expression for the $\sigma\begin{Bmatrix} p & q & s & t \\ p'0 & & s'0 \end{Bmatrix}^{(a)}$ collision integrals. For $q' = t' = 0$, equation (I.2-7) can be written

$$\sigma\begin{Bmatrix} p & q & s & t \\ p'0 & & s'0 \end{Bmatrix}^{(a)} = (-1)^{q+a+p}\ \delta(p'|a)\alpha^{-1}(a)\alpha(q)\alpha(q0q)^{1/2} \sum_{\substack{\ell n \\ \ell' n'}} \alpha(q\ell\ell')^{1/2}$$

$$\times\ [1 + (-1)^{\ell'}]\ I^{(q)}_{\ell n\ell' n';psp's'}\ \sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell'0 & & n'0 \end{Bmatrix}_q \ . \qquad \text{(I.7-6)}$$

In detail this becomes

$$\sigma\begin{Bmatrix} p & q & s & t \\ p'0 & & s'0 \end{Bmatrix}^{(a)} = (-1)^{a+p}\ \alpha^{-1}(a)\ \delta(p'|a)\ \frac{\hbar^2\pi^{3/2}}{4\mu k_B T} \sum_{\substack{\ell n \\ \ell' n'}} [1 + (-1)^{\ell'}]$$

$$\times\ I^{(q)}_{\ell n\ell' n';psp's'} \Bigg\{ [\sum_{\lambda} \alpha^2(\lambda)\alpha(\ell)\delta(\ell q t|\ell' 00) \int d\gamma\ \gamma\ R_{n\ell}(\gamma)\ R_{n'\ell}(\gamma)]$$

$$- 2\Bigg[(i)^{q+\ell+\ell'}\ \alpha(\ell\ell')\left[\frac{\Gamma(n+1)\ \Gamma(n'+1)}{\Gamma(n+\ell+3/2)\Gamma(n'+\ell'+3/2)}\right]^{1/2} (8\pi^2)^{-2}$$

$$\times \sum_{\substack{j_a' j_b' \\ \lambda\lambda'}} \alpha^2(\lambda\lambda')(p_{j_a' j_b'}) \sum_{\alpha\beta} (i)^{\alpha-\beta} \begin{pmatrix} \lambda & \lambda' & \ell' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell & q & \ell' \\ 0 & \beta & -\beta \end{pmatrix}$$

$$\times \int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n'}^{\ell'+1/2}(\gamma^2) \iint dS_a dS_b\ S^*(j_a' j_b' \lambda\lambda' | S_a S_b)$$

$$\times\ I_a(q-\alpha)D^q_{\alpha\beta}(S_a)E^*_{ab}(\lambda\lambda'\ell';-\beta)C^*_{ab}(\ell qnt)\ S(j_a' j_b' \lambda|S_a S_b)\Bigg]\Bigg\} \ , \qquad \text{(I.7-8)}$$

a result that is useful in considering some special cases of the collision integrals.

For $p = s = 0$, the quantity $I^{(q)}_{\ell n \ell' n';00p's'}$ is found to be

$$I^{(q)}_{\ell n \ell' n';00p's'} = \left(\frac{1}{\sqrt{2}}\right)^{2s'+p'} \delta_{\ell n,00}\, \delta_{\ell' n',p's'}\, \delta_{\ell',q}$$

$$= \left(\frac{1}{\sqrt{2}}\right)^{2s'+q} \delta(\ell n \ell' n' | 00qs')\, \delta(p'|q) \,, \qquad (1.7\text{-}9a)$$

yielding

$$\sigma\begin{Bmatrix} 0 & q & 0 & t \\ p' & 0 & s' & 0 \end{Bmatrix}^{(a)} = \delta(p'|a)\, \delta(p'|q)\, \Omega(q0q)[1 + (-1)^q] \left(\frac{1}{\sqrt{2}}\right)^{2s'+q}$$

$$\times\ \sigma'\begin{Bmatrix} 0 & q & 0 & t \\ q & 0 & s' & 0 \end{Bmatrix}_q \,. \qquad (1.7\text{-}9b)$$

In comparison, for $p = 1$, $s = 0$, it is found that

$$I^{(q)}_{\ell n \ell' n';10p's'} = \left(\frac{1}{\sqrt{2}}\right)^{2+2s'+q} \delta(\ell n \ell' n' | 00qs')\, \delta(p'|q+1)$$

$$\cdot \left[\frac{(q+1)(2q+2s'+3)}{(2q+1)}\right]^{1/2} - \left(\frac{1}{\sqrt{2}}\right)^{2s'+q} \delta(\ell n \ell' n' | 00q(s'-1))\, \delta(p'|q-1)$$

$$\cdot \left[\frac{2qs'}{(2q+1)}\right]^{1/2} + \delta(\ell n|10)\, I^{(q)}_{10\ell' n';10p's'} \,, \qquad (1.7\text{-}10a)$$

and

$$\sigma\begin{pmatrix}1 & q & 0 & t\\ p' & 0 & s' & 0\end{pmatrix}^{(a)} = \delta(p'|a)\Omega(q0q)[1+(-1)^q]\left(\frac{1}{\sqrt{2}}\right)^{2s'+q}$$

$$\times\left\{\tfrac{1}{2}\delta(p'|q+1)\left[\frac{(q+1)(2q+2s'+3)}{2q+3}\right]^{1/2}\sigma'\begin{pmatrix}0 & q & 0 & t\\ q & 0 & s' & 0\end{pmatrix}_q\right.$$

$$\left.+\ \delta(p'|q-1)\left[\frac{2qs'}{(2q-1)}\right]^{1/2}\sigma'\begin{pmatrix}0 & q & 0 & t\\ q & 0 & s'-1 & 0\end{pmatrix}_q\right\}, \qquad (I.7\text{-}10b)$$

since parity considerations demand that $\ell+\ell'$ be even.[4]

Solving the above expressions for $\sigma'\begin{pmatrix}0 & q & 0 & t\\ q & 0 & s' & 0\end{pmatrix}_q$:

$$\sigma'\begin{pmatrix}0 & q & 0 & t\\ q & 0 & s' & 0\end{pmatrix}_q = \Omega(q0q)^{-1}\,[1+(-1)^q]^{-1}\,(\sqrt{2})^{2s'+q}\sigma\begin{pmatrix}0 & q & 0 & t\\ q & 0 & s' & 0\end{pmatrix}^{(q)} \qquad (I.7\text{-}11a)$$

$$= \Omega(q0q)^{-1}\,[1+(-1)^q]^{-1}\,(\sqrt{2})^{2s'+q}$$

$$\times\left\{2\left[\frac{2q+3}{(q+1)(2q+2s'+3)}\right]^{1/2}\sigma\begin{pmatrix}1 & q & 0 & t\\ q+1 & 0 & s' & 0\end{pmatrix}^{(q+1)}\right\} \qquad (I.7\text{-}11b)$$

$$= \Omega(q0q)^{-1}\,[1+(-1)^q]^{-1}\,(\sqrt{2})^{2s'+q}$$

$$\times\left\{-2\left[\frac{2q-1}{2q(s'+1)}\right]^{1/2}\sigma\begin{pmatrix}1 & q & 0 & t\\ q-1 & 0 & s'+1 & 0\end{pmatrix}^{(q-1)}\right\}. \qquad (I.7\text{-}11c)$$

It follows that

$$2\left[\frac{2q+3}{(q+1)(2q+2s'+3)}\right]^{1/2} \sigma\begin{Bmatrix} 1 & q & 0 & t \\ q+1 & 0 & s' & 0 \end{Bmatrix}^{(q+1)} - \sigma\begin{Bmatrix} 0 & q & 0 & t \\ q & 0 & s' & 0 \end{Bmatrix}^{(q)}$$

$$= -2\left[\frac{2q-1}{2q(s'+1)}\right]^{1/2} \sigma\begin{Bmatrix} 1 & q & 0 & t \\ q-1 & 0 & s'+1 & 0 \end{Bmatrix}^{(q-1)} , \qquad \text{(I.7-12)}$$

analogous to CMS-43.

Other interesting relations are obtained by considering the case $q = q' = t' = 0$. Equation (I.7-6) becomes

$$\sigma\begin{Bmatrix} p & 0 & s & t \\ p' & 0 & s' & 0 \end{Bmatrix}^{(a)} = (-1)^{a+p}\, \delta(p'|a)\,\alpha^{-1}(a) \sum_{\substack{\ell n \\ \ell' n'}} \alpha(0\ell\ell')^{1/2}\, [1 + (-1)^{\ell'}]$$

$$\times\, I^{(0)}_{\lambda n\ell' n';psp's'}\, \sigma'\begin{Bmatrix} \ell & 0 & n & t \\ \ell' & 0 & n' & 0 \end{Bmatrix}_0 . \qquad \text{(I.7-13)}$$

Examination of $I^{(0)}_{\lambda n\ell' n';psp's'}$ reveals that

$$I^{(0)}_{\lambda n\ell' n';psp's'} = \pi^{-1/2}\, (1/2)^{s+s'+p}\, \delta_{n',n+s'-s}$$

$$\times \left[\frac{s!\,s'!\,\Gamma(p+s+3/2)\,\Gamma(p+s'+3/2)\,(2\lambda+1)(2p+1)}{n!\,n'!\,\Gamma(\lambda+n+3/2)\,\Gamma(\lambda+n'+3/2)}\right]^{1/2}$$

$$\times \sum_{L} \frac{(2L+1)}{\left(s-n+\frac{p-\lambda-L}{2}\right)!\,\left(s-n+\frac{3+p-\ell+L}{2}\right)} \begin{pmatrix} p & \lambda & L \\ 0 & 0 & 0 \end{pmatrix}^2 \delta(\lambda p|\ell' p') ,$$

(I.7-14)

which leads to

$$\sigma\begin{Bmatrix} p & 0 & s & t \\ p' & 0 & s' & 0 \end{Bmatrix}^{(a)} = \delta(p'|p)\ \delta(p|a)\ \alpha^{-1}(a) \sum_{\ell n} \Omega(0\ell\ell)^{1/2}$$

$$\times\ [1 + (-1)^{\ell}]\ \frac{\pi^{1/2}}{2}\ (1/2)^{s+s'+p} \left[\frac{s!s'!\Gamma(p+s+3/2)\Gamma(p+s'+3/2)(2\ell+1)2p+1)}{n!(n+s'-s)!\Gamma(\ell+n+3/2)\Gamma(\ell+n+s'-s+3/2)}\right]^{1/2}$$

$$\times \sum_{L} \frac{(2L+1)}{\left(s - n + \frac{p-\ell-L}{2}\right)!\,\Gamma\left(s - n + \frac{3+p-\ell+L}{2}\right)} \begin{pmatrix} p & \ell & L \\ 0 & 0 & 0 \end{pmatrix}^2 \sigma'\begin{Bmatrix} \ell & 0 & n & t \\ \ell & 0 & n+s'-s & 0 \end{Bmatrix}_0 ,$$

(I.7-15)

with

$$\sigma'\begin{Bmatrix} \ell & 0 & n & t \\ \ell & 0 & n-\bar{s} & 0 \end{Bmatrix}_0 = \frac{\hbar^2\pi^{3/2}}{4\mu k_B T}\ \Omega(0\ell\ell)^{-1/2}\ \alpha(\ell)$$

$$\times \left\{ \left[\sum_{\lambda} \alpha^2(\lambda)\ \delta(t|0) \int d\gamma\gamma\ R_{n\ell}(\gamma)\ R_{n-\bar{s},\ell}(\gamma)\right] \right.$$

$$- 2\left[\frac{\Gamma(n+1)\ \Gamma(n-\bar{s}+1)}{\Gamma(n+\ell+3/2)\Gamma(n-\bar{s}+\ell+3/2)}\right]^{1/2} (8\pi^2)^{-2} \left[\sum_{\substack{j_a' j_b' \\ \lambda\lambda'}} \alpha^2(\lambda\lambda')(p_{j_a' j_b'}) \begin{pmatrix} \lambda & \lambda' & \ell \\ 0 & 0 & 0 \end{pmatrix}\right.$$

$$\times \int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n-\bar{s}}^{\ell+1/2}(\gamma^2) \iint dS_a\, dS_b\ S^{*}(j_a' j_b' \lambda' | S_a S_b)$$

$$\left.\left.\times\ E_{ab}^{*}(\ell,0)\ C_{ab}^{*}(\ell 0 n t)\ S(j_a' j_b' \lambda | S_a S_b)\right]\right\} . \qquad \text{(I.7-16)}$$

Equation (I.7-15) can now be rewritten

$$\sigma\begin{pmatrix} p & 0 & s & t \\ p' & 0 & s' & 0 \end{pmatrix}^{(a)} = \delta(p'|p)\delta(p|a)(\tfrac{1}{2})^{s+s'+p}[s!s'!\Gamma(p+s+\tfrac{3}{2})\Gamma(p+s'+\tfrac{3}{2})]^{1/2}$$

$$\times \sum_{\ell n L} \alpha^2(\ell)[1+(-1)^{\ell}][\Gamma(\ell+n+\tfrac{3}{2})\Gamma(\ell+n-\bar{s}+\tfrac{3}{2})]^{-1}$$

$$\times \frac{\alpha^2(L)\begin{pmatrix} p & \ell & L \\ 0 & 0 & 0 \end{pmatrix}^2}{\left[s-n+\frac{p-\ell-L}{2}\right]!\,\Gamma\left[s-n+\frac{3+p-\ell+L}{2}\right]}$$

$$\times \frac{\hbar^2\pi^2}{4\mu k_B T}\Bigg\{[\sum_{\lambda} \alpha^2(\lambda)\delta(t|0)\int d\gamma\ \gamma^{2\ell+1}\ e^{-\gamma^2}\ L_n^{\ell+1/2}(\gamma^2)L_{n-\bar{s}}^{\ell+1/2}(\gamma^2)]$$

$$-\Bigg[\sum_{\substack{j_a'j_b' \\ \lambda\lambda'}} \alpha^2(\lambda\lambda')(p_{j_a'j_b'})\begin{pmatrix} \lambda & \lambda' & \ell \\ 0 & 0 & 0 \end{pmatrix}\int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n-\bar{s}}^{\ell+1/2}(\gamma^2)$$

$$\times (8\pi^2)^{-2}\iint dS_a dS_b\ \mathcal{S}^{\star}(j_a'j_b'\lambda'|S_aS_b)$$

$$\times F_{ab}^{\star}(\ell,0)\ C_{ab}^{\star}(\ell 0 n t)\ \mathcal{S}(j_a'j_b'\lambda|S_aS_b)\Bigg]\Bigg\}\ . \tag{I.7-17}$$

Defining two new quantities,

$$G(ps:\ell n) \equiv \sum_{L} \frac{\alpha^2(L)[1+(-1)^{\ell}]\begin{pmatrix} p & \ell & L \\ 0 & 0 & 0 \end{pmatrix}^2}{2\left[s-n+\frac{p-\ell-L}{2}\right]!\,\Gamma\left[s-n+\frac{3+p-\ell+L}{2}\right]} \tag{I.7-18}$$

and

$$\sigma[\ell n;\bar{s}t] = \frac{\hbar^2\ \pi^2}{2\mu k_B T}\alpha^2(\ell)[\Gamma(\ell+n+3/2)\Gamma(\ell+n-\bar{s}+3/2)]^{-1}$$

$$\times\Bigg\{[\sum_{\lambda}\alpha^2(\lambda)\delta(t|0)\int d\gamma\ \gamma^{2\ell+1}\ e^{-\gamma^2}\ L_n^{\ell+1/2}(\gamma^2)\ L_{n-\bar{s}}^{\ell+1/2}(\gamma^2)]$$

$$-\Bigg[\sum_{\substack{j_a'j_b'\\ \lambda\lambda'}}\alpha^2(\lambda\lambda')(p_{j_a'j_b'})\begin{pmatrix}\lambda & \lambda' & \ell\\ 0 & 0 & 0\end{pmatrix}\int d\gamma\ \gamma^{\ell+1}\ e^{-\gamma^2}\ L_{n-\bar{s}}^{\ell+1/2}(\gamma^2)$$

$$\times(8\pi^2)^{-2}\iint dS_a dS_b\ S^*(j_a'j_b'\lambda'|S_aS_b)E_{ab}^*(\ell,0)C_{ab}^*(\ell 0nt)S(j_a'j_b'\lambda|S_aS_b)\Bigg]\Bigg\}\ ,$$

(I.7-19)

allows (I.7-17) to be written in the simple form:

$$\sigma\begin{pmatrix}p & 0 & s & t\\ p' & 0 & s' & 0\end{pmatrix}^{(a)} = \delta(p'|p)\delta(p|a)(1/2)^{s+s'+p}[s!s'!\Gamma(p+s+3/2)\Gamma(p+s'+3/2)]^{1/2}$$

$$\times\sum_{\ell n}G(ps;\ell n)\ \sigma[\ell n;\bar{s}t]\ . \qquad (I.7\text{-}20)$$

The usefulness of the above expression is apparent in the treatment of the following example. The scalar, $\sigma\binom{1010}{1010}^{(1)}$, can be written

$$\sigma\binom{1010}{1010}^{(1)} = 1/8\ \Gamma(7/2)\sum_{\ell n}G(11;\ell n)\ \sigma[\ell n;00]\ , \qquad (I.7\text{-}21a)$$

with

$$G(11;\ell n) = \frac{\delta(\ell n|00)}{\Gamma(7/2)} + \frac{\delta(\ell n|01)}{\Gamma(7/2)} + \frac{2}{5}\frac{\delta(\ell n|20)}{\Gamma(7/2)}\ . \qquad (I.7\text{-}21b)$$

Then, since $\sigma[00;00] = 0$,

$$\sigma\binom{1010}{1010}^{(1)} = \frac{5}{16}\,\sigma[01;00] + \frac{1}{8}\,\sigma[20;00] \,. \qquad \text{(I.7-21c)}$$

Similar treatment of $\sigma\binom{2000}{2000}^{(2)}$ and $\sigma\binom{0010}{0010}^{(0)}$ yields

$$\sigma\binom{2000}{2000}^{(2)} = \frac{3}{16}\,\sigma[20;00] \qquad \text{(I.7-22)}$$

and

$$\sigma\binom{0010}{0010}^{(0)} = \frac{3}{8}\,\sigma[01;00] \,, \qquad \text{(I.7-23)}$$

from which it is apparent that

$$\sigma\binom{1010}{1010}^{(1)} = \frac{5}{6}\,\sigma\binom{0010}{0010}^{(0)} + \frac{2}{3}\,\sigma\binom{2000}{2000}^{(2)} \,. \qquad \text{(I.7-24)}$$

This is analogous to CMS-47.

Other special cases could be examined to obtain other relations among the $\sigma\begin{pmatrix} p & q & s & t \\ p' & q' & s' & t' \end{pmatrix}^{(a)}$ collision integrals. The examples treated in this section are representative of the types of manipulations that can be done once certain of the indices of the collision integrals are restricted in some fashion. The relations that can be found make it possible to evaluate collision integrals based upon information obtained in the detailed treatment of other collision integrals, at a great savings in time and effort. Furthermore, though the relations of this section apply to

single component diatomic collision partners, the results for the $\sigma'\begin{pmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{pmatrix}_k$ and $\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{pmatrix}_k$ collision integrals may be generalized to other collision pairs. This becomes important in the later portions of this thesis.

I.8 Summary

In summary, the first section of this part, essentially a review of Hunter's work, provides the motivation for the reduction of the $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ relative momentum collision integrals of the remainder of Part I. In section I.2, the relationship between the relative momentum collision integrals and the kinetic theory cross sections, $\sigma'(\ell n j_a j_b q | \ell' n' j_a' j_b' q')_k$ and $\sigma''(\ell n j_a j_b q | \ell' n' j_b' j_a' q')_k$, of Hunter and Snider is established. In that section, the $\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}$ scalars, introduced in section I.1, are expressed in terms of the relative momentum collision integrals. In sections I.3 and I.5, the connection between the work of Hunter and Snider and that of Curtiss and co-workers is made. In these two sections, the relative momentum collision integrals are expressed in terms of the reduced scattering matrix, $S(j_a' j_b' \lambda | s_a s_b)$.

Sections I.1, I.2, I.3, and I.5 set the groundwork necessary for the important results of sections I.4 and I.6. The new results of Part I are presented in these two sections; the angle derivative operators, $C_{ab}(\ell qnt)$, $F_{ab}(\lambda\lambda'\ell';-\beta'-\beta)$, $E_a(q'j_a';-\alpha')$, $E_b(q'j_b';\alpha')$, and $I_a(q-\alpha)$ are introduced and a number of the summations and angle integrations carried out. In this manner, $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ is simplified from a sixteen-fold summation and twelve-fold angle integration to a summation over eight indices

and an integration over six angles, while $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ is reduced from a summation over nineteen indices and an integration over twelve angles to a similar eight-fold summation and six-fold angle integration.

It is shown in section I.7 that the restriction of $q' = t' = 0$ leads to a number of interesting relations among the relative momentum collision integrals and the $\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}$ scalars. One of the most important of these is the equality of $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{Bmatrix}_k$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & 0 & n' & 0 \end{Bmatrix}_k$.

The simplifications of $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k$ in sections I.4 and I.6 provide a major first step toward calculation of the transport properties of a dilute single component diatomic gas in the presence of an applied magnetic field. Though within the realm of possibility, such a calculation proves extememly difficult due to the dependence of the intermolecular potential on three orientation angles for a diatomic-diatomic collision. On the other hand, the interaction potential for an atom-diatom collision is a function of a single angle. Calculations of collision cross sections for atom-diatom collisions and transport properties of a binary atom-diatom mixture have recently been completed[13] by R. Wood for a gas of argon atoms with a small molecular nitrogen component. This calculation involves a gas mixture in the absence of a field. The remainder of this work develops the algebraic groundwork for

the calculation of the transport properties for a similar system in the presence of a magnetic field.

In order to carry out such a calculation, it is first necessary to generalize the development presented in Part I to a binary gas mixture. This is accomplished in Part II. Then, in Part III, the general binary gas mixture is restricted to an atom-diatom mixture and expressions for the spherical components of the viscosity tensor in the presence of an applied magnetic field are obtained.

Appendix I.A Explicit Expressions for $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$ and $I_a(q\mu_2)$ with $q = 0,1,$ and 2

The $I(q\mu_2;\kappa j_a'\mu_1\mu_2')$ sums defined by equation (I.4-10a) are evaluated using recursion relations among the 3-j coefficients.[8,9] Their values for $q = 0,1,$ and 2 are

$$I(00;\kappa j_a'\mu_1\mu_2') = \delta_{\mu_2',-\mu_1} , \tag{I.A-1}$$

$$I(11;\kappa j_a'\mu_1\mu_2') = \delta_{\mu_2',-\mu_1+1}\ \lambda_-(\kappa\mu_1) + \delta_{\mu_2',-\mu_1}\ \lambda_-(j_a'\mu_1) , \tag{I.A-2}$$

$$I(10;\kappa j_a'\mu_1\mu_2') = 0 , \tag{I.A-3}$$

$$I(1,-1;\kappa j_a'\mu_1\mu_2') = -\delta_{\mu_2',-\mu_1-1}\ \lambda_+(\kappa\mu_1) - \delta_{\mu_2',-\mu_1}\ \lambda_+(j_a'\mu_1) , \tag{I.A-4}$$

$$\begin{aligned} I(22;\kappa j_a'\mu_1\mu_2') = {} & \tfrac{1}{2}\delta_{\mu_2',-\mu_1+2}\ \lambda_-(\kappa\mu_1)\lambda_-(\kappa\mu_1-1) \\ & + \delta_{\mu_2',-\mu_1+1}\ \lambda_-(\kappa\mu_1)\lambda_-(j_a'\mu_1-1) \\ & + \tfrac{1}{2}\delta_{\mu_2',-\mu_1}\ \lambda_-(j_a'\mu_1)\lambda_-(j_a'\mu_1-1) , \end{aligned} \tag{I.A-5}$$

$$I(21;\kappa j_a'\mu_1\mu_2') = -\tfrac{1}{2}\delta_{\mu_2',-\mu_1+1}\ \lambda_-(\kappa\mu_1) - \tfrac{1}{2}\delta_{\mu_2',-\mu_1}\ \lambda_-(j_a'\mu_1) \tag{I.A-6a}$$

$$= -\tfrac{1}{2}\ I(11;\kappa j_a'\mu_1\mu_2') , \tag{I.A-6b}$$

$$I(20;\kappa j_a'\mu_1\mu_2') = -\frac{1}{\sqrt{6}}\delta_{\mu_2',-\mu_1}[\kappa(\kappa+1) + j_a'(j_a'+1) - 2\mu_1^2]$$

$$-\frac{1}{\sqrt{6}}\delta_{\mu_2',-\mu_1+1}\lambda_-(\kappa\mu_1)\lambda_-(j_a'\mu_1)$$

$$-\frac{1}{\sqrt{6}}\delta_{\mu_2',-\mu_1-1}\lambda_+(\kappa\mu_1)\lambda_+(j_a'\mu_1)\ , \qquad \text{(I.A-7)}$$

$$I(2,-1;\kappa j_a'\mu_1\mu_2') = -\tfrac{1}{2}\delta_{\mu_2',-\mu_1-1}\lambda_+(\kappa\mu_1) - \tfrac{1}{2}\delta_{\mu_2',-\mu_1}\lambda_+(j_a'\mu_1) \qquad \text{(I.A-8a)}$$

$$= [illegible]\ I(2,-1;\kappa j_a'\mu_1\mu_2')\ , \qquad \text{(I.A-8b)}$$

and

$$I(2,-2;\kappa j_a'\mu_1\mu_2') = [illegible]\ \delta_{\mu_2',-\mu_1-2}\lambda_+(\kappa\mu_1)\lambda_+(\kappa\mu_1+1)$$

$$+ \delta_{\mu_2',-\mu_1-1}\lambda_+(\kappa\mu_1)\lambda_+(j_a'\mu_1+1)$$

$$+ [illegible]\ \lambda_+(j_a'\mu_1)\lambda_+(j_a'\mu_1+1)\ , \qquad \text{(I.A-9)}$$

where

$$\lambda_\pm(l,\mu) = [l(l+1) - \mu(\mu\pm1)]^{1/2}\ .$$

The corresponding [illegible], $I_a(q,\mu)$, are constructed in such a manner that th[illegible] equation (1.4-13). For $q = 0,1$, and 2 they are

$$I_a(0,0) = 1\ , \qquad \text{(I.A-10)}$$

$$I_a(1,1) = -\ [illegible]\ ,\hbar^{-1}L_z^{(a)})\ , \qquad \text{(I.A-11)}$$

$$I_a(1,0) = 0 \ , \tag{I.A-12}$$

$$I_a(1,-1) = [illegible] \hbar^{-1} L^{(a)}) \ , \tag{I.A-13}$$

$$I_a(2,2) = -\frac{1}{\hbar} [illegible] (j_a', \hbar^{-1} L_3^{(a)}) L_+^{(a)}$$

$$+ \tfrac{1}{2} [illegible] \hbar^{-1} L_3^{(a)} + 1) \ , \tag{I.A-14}$$

$$I_a(2,1) = [illegible] \tag{I.A-15}$$

$$I_a(2,0) = [illegible] - 2\hbar^{-2} L^{(a)2}]$$

$$+ [illegible] \hbar^{-1} L^{(a)}) + \frac{i}{3\hbar} L_-^{(a)} \ldots (j_a', \hbar^{-1} L_3^{(a)}) \ , \tag{I.A-16}$$

$$I_a(2,-1) = \tfrac{1}{2} [illegible] \tag{I.A-17}$$

and

$$I_a(2,-2) = [illegible] (j_a', \hbar^{-1} L_3^{(a)}) L_-^{(a)}$$

$$+ [illegible] \hbar^{-1} L_3^{(a)} - 1) \ , \tag{I.A-18}$$

where $L^{(a)2}$ [illegible] and $L_1^{(a)}$, $L_2^{(a)}$, $L_3^{(a)}$, and $L_+^{(a)}$ are [illegible]

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PART II.

A BINARY GAS MIXTURE IN AN APPLIED MAGNETIC FIELD

II.1 Generalization of the Linearized Waldmann-Snider Equation to Binary Gas Mixtures

In Part I, the linearized Waldmann-Snider equation [1,2] is used to obtain the transport properties of a single component diatomic gas in an applied magnetic field. The starting point of the development is

$$\frac{\partial f^{(0)}}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f^{(0)} = -f^{(0)}(\mathcal{R} + iL)\phi \qquad \text{(II.1-1)}$$

where $\frac{\mathbf{p}}{m}$ is the velocity, $f^{(0)}$ is the equilibrium Maxwell-Boltzmann distribution function-density operator, [2] normalized [3] such that

$$n(\underline{r},t) = \mathrm{Tr}\int d\underline{p}\, f^{(0)} , \qquad (II.1\text{-}2a)$$

$$\rho\underline{v}_0(\underline{r},t) = \mathrm{Tr}\int d\underline{p}\, f^{(0)}\underline{p} , \qquad (II.1\text{-}2b)$$

and

$$U^{(0)}(\underline{r},t) = U^{(0)}_{trans}(\underline{r},t) + U^{(0)}_{int}(\underline{r},t)$$

$$(II.1\text{-}2c)$$

$$= \frac{1}{n}\mathrm{Tr}\int d\underline{p}\, f^{(0)}\, [\tfrac{m}{2}(\tfrac{\underline{p}}{m} - \underline{v}_0)^2 + H'] ,$$

and ϕ is the perturbation operator occurring in the perturbation expansion of the singlet distribution function-density operator, f ,

$$f = f^{(0)}\,(1+\phi+\ldots) . \qquad (II.1\text{-}3)$$

In the above, $\mathcal{R}$ and L are the linearized Waldmann-Snider collision superoperator and the Larmor precession superoperator introduced in Part I. The quantities n, $\underline{v}_0$, and $U^{(0)}$ are the local values of the macroscopic number density, mass-average velocity, and energy density, respectively. ρ is the mass density [illegible], and H' is the internal state Hamiltonian in the absence of an external field. The traces are taken over internal states. The equilibrium distribution, $f^{(0)}$, then takes the form

$$f^{(0)} = (\tfrac{n}{Q})\, [2\pi m k_B T]^{-3/2} \exp[-W^2 - \frac{H'}{k_B T}] , \qquad (II.1\text{-}4)$$

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where m is the molecular mass, $\underline{W} = (2mk_BT)^{-1/2}(\underline{p} - m\underline{v}_0)$ is the reduced peculiar velocity, and Q is the internal state partition function.

The generalization of equation (II.1-1) is accomplished in direct analogy to the generalization of the single component Boltzmann equation proposed by Wang Chang and Uhlenbeck [4] and discussed by Monchick, Yun, and Mason. [3] In the absence of an external field, the linearized Waldmann-Snider equation for a binary mixture is written [3,5]

$$\frac{\partial f_k^{(0)}}{\partial t} + \frac{\underline{p}_k}{m_k} \cdot \underline{\nabla} f_k^{(0)} = -f_k^{(0)} \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}\phi_k + \mathcal{R}''_{k\ell}\phi_\ell) \,, \tag{II.1-5}$$

where

$$\mathcal{R}'_{k\ell}\phi_k = -(2\pi)^4 h^2 \mathrm{Tr}_\ell \int d\underline{p}_\ell f_\ell^{(0)} [\{\iint d\underline{p}'_\ell d\underline{p}_k <\mu_{k\ell}\underline{g}_{k\ell}|t|\mu_{k\ell}\underline{g}'_{k\ell}>\phi'_k$$

$$\times <\mu_{k\ell}\underline{g}'_{k\ell}|\delta(E)t^\dagger|\mu_{k\ell}\underline{g}_{k\ell}>\delta(\underline{p}_k+\underline{p}_\ell-\underline{p}'_k-\underline{p}'_\ell)\} \tag{II.1-6a}$$

$$+ \frac{1}{(2\pi i)}\{<\mu_{k\ell}\underline{g}_{k\ell}|t|\mu_{k\ell}\underline{g}_{k\ell}> \phi_k - \phi_k <\mu_{k\ell}\underline{g}_{k\ell}|t^\dagger|\mu_{k\ell}\underline{g}_{k\ell}>\}] \,,$$

and

$$\mathcal{R}''_{k\ell}\phi_\ell = -(2\pi)^4\hbar^2 \mathrm{Tr}_\ell \int d\underline{p}_\ell f_\ell^{(0)} [\{\iint d\underline{p}'_\ell d\underline{p}'_k \langle \mu_{k\ell}\underline{g}_{k\ell}|t|\mu_{k\ell}\underline{g}'_{k\ell}\rangle \phi'_\ell$$

$$\times \langle \mu_{k\ell}\underline{g}'_{k\ell}|\delta(E)t^\dagger|\mu_{k\ell}\underline{g}_{k\ell}\rangle \delta(\underline{p}_k+\underline{p}_\ell-\underline{p}'_k-\underline{p}'_\ell)\} \qquad \text{(II.1-6b)}$$

$$+\frac{1}{(2\pi i)}\{\langle \mu_{k\ell}\underline{g}_{k\ell}|t|\mu_{k\ell}\underline{g}_{k\ell}\rangle \phi_\ell - \phi_\ell \langle \mu_{k\ell}\underline{g}_{k\ell}|t^\dagger|\mu_{k\ell}\underline{g}_{k\ell}\rangle\}] \ .$$

In the above, t is the transition operator,[6] $\underline{g}'_{k\ell}$ and $\underline{g}_{k\ell}$ are the relative velocities of particle k and particle ℓ before and after collision, and $\mu_{k\ell}$ is the reduced mass of particles k and ℓ. Addition of (II.1-6a) and (II.1-6b) yields

$$\mathcal{R}'_{k\ell}\phi_k + \mathcal{R}''_{k\ell}\phi_\ell = -(2\pi)^4\hbar^2 \mathrm{Tr}_\ell \int d\underline{p}_\ell f_\ell^{(0)} [\{\iint d\underline{p}'_\ell d\underline{p}'_k \langle \mu_{k\ell}\underline{g}_{k\ell}|t|\mu_{k\ell}\underline{g}'_{k\ell}\rangle (\phi'_k+\phi'_\ell)$$

$$\times \langle \mu_{k\ell}\underline{g}'_{k\ell}|\delta(E)t^\dagger|\mu_{k\ell}\underline{g}_{k\ell}\rangle \delta(\underline{p}_k+\underline{p}_\ell-\underline{p}'_k-\underline{p}'_\ell)\} \qquad \text{(II.1-7)}$$

$$+\frac{1}{(2\pi i)}\{\langle \mu_{k\ell}\underline{g}_{k\ell}|t|\mu_{k\ell}\underline{g}_{k\ell}\rangle (\phi_k+\phi_\ell) - (\phi_k+\phi_\ell)$$

$$\times \langle \mu_{k\ell}\underline{g}_{k\ell}|t^\dagger|\mu_{k\ell}\underline{g}_{k\ell}\rangle\}] \ ,$$

the right hand side of which is clearly the generalization of $\mathcal{R}\phi$ of Ref. 7 to multicomponent systems. The essential difference between $(\mathcal{R}'_{k\ell}\phi_k + \mathcal{R}''_{k\ell}\phi_\ell)$ and $\mathcal{R}\phi$ lies in the fact that in a multicomponent system, collision partners may be of different species.

The extension of (II.1-5) to include the effect of an external magnetic field is immediate. For a binary mixture,

$$\frac{\partial f_k^{(0)}}{\partial t} + \frac{\underline{p}_k}{m_k} \cdot \underline{\nabla} f_k^{(0)} = -f_k^{(0)} \left[i L_k \phi_k + \sum_{\ell=1}^{2} \left(\mathcal{R}_{k\ell} \phi_k + \mathcal{R}'_{k\ell} \phi_\ell \right) \right] , \tag{II.1-8}$$

where L_k is the Larmor precession superoperator[8] for species k :

$$L_k \phi_k = -(\omega_L)_k \, [(J_z)_k, \phi_k] \, . \tag{II.1-9}$$

In the following section, equation (II.1-8) is examined in detail and tensor equations are developed for the perturbation operator, ϕ_k , of a binary gas mixture. This allows the tensor equations for the transport properties to be obtained in section II.3 In section II.4, scalar equations for the transport properties are obtained from the tensor equations. These are written in terms of collisional scalars analogous to the $\sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}(a)$ scalars of Part I. The new scalars are expressed in terms of binary mixture relative momentum collision integrals in section II.5, drawing to a close the formal treatment of a binary gas mixture in an applied magnetic field.

II.2 The Perturbation Operator of a Binary Mixture

The generalization of the linearized Waldmann-Snider equation to binary gas mixtures, equation (II.1-8), can also be written in the compact form

$$-\psi_k = iL_k\phi_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}\phi_k + \mathcal{R}''_{k\ell}\phi_\ell) \;. \qquad \text{(II.2-1)}$$

Equations (II.1-8) and (II.2-1) are obtained from the treatment of the following perturbation expansion of the distribution function-density operator, f_k :

$$f_k = f_k^{(0)} (1+\phi_k+\ldots) \;. \qquad \text{(II.2-2)}$$

Here, as in the previous equations, $f_k^{(0)}$ is the equilibrium Maxwell-Boltzmann distribution function-density operator. It is normalized [3] such that

$$n_k(\underline{r},t) = \mathrm{Tr}_k \int f_k^{(0)} \, d\underline{p}_k \qquad \text{(II.2-3a)}$$

$$1/\rho \sum_k \mathrm{Tr}_k \int f_k^{(0)} \, \underline{p}_k \, d\underline{p}_k = \underline{v}_0(\underline{r},t) \;, \qquad \text{(II.2-3b)}$$

where

$$\rho = \sum_k n_k m_k \;, \qquad \text{(II.2-3c)}$$

and

$$1/\rho \sum_k \mathrm{Tr}_k \int f_k^{(0)} \left[\frac{m_k}{2}\left(\frac{\underline{p}_k}{m_k} - \underline{v}_0\right)^2 + H_k'\right] d\underline{p}_k =$$

$$U_{tr}^{(0)}(\underline{r},t) + U_{int}^{(0)}(\underline{r},t) = U^{(0)}(\underline{r},t) , \qquad \text{(II.2-3d)}$$

in which H_k' is the internal state Hamiltonian neglecting interactions with an applied field.

The requirement that n_k , $\underline{v}_0$, and $U^{(0)}$ be local values of the macroscopic number density, mass-average velocity, and energy density, respectively, demands that the following auxiliary conditions be satisfied:

$$0 = \mathrm{Tr}_k \int f_k^{(0)} \phi_k \, d\underline{p}_k , \qquad \text{(II.2-4a)}$$

$$0 = \sum_k \mathrm{Tr}_k \int f_k^{(0)} \phi_k \left[\underline{p}_k - m_k \underline{v}_0\right] d\underline{p}_k , \qquad \text{(II.2-4b)}$$

and

$$0 = \sum_k \mathrm{Tr}_k \int f_k^{(0)} \phi_k \left[W_k^2 + \frac{H'_k}{k_B T}\right] d\underline{p}_k , \qquad \text{(II.2-4c)}$$

where

$$\underline{W}_k = \left(\frac{m_k}{2k_B T}\right)^{1/2} \underline{V}_k = \left(\frac{m_k}{2k_B T}\right)^{1/2} \left[\frac{\underline{p}_k}{m_k} - \underline{v}_0\right] . \qquad \text{(II.2-4d)}$$

Equations (II.2-3a - II.2-3d) are satisfied if

$$f_k^{(0)} = \left(\frac{n_k}{Q_k}\right)\left[2\pi m_k k_B T\right]^{-3/2} \exp\left[-W_k^2 - \frac{H'_k}{k_B T}\right] , \qquad \text{(II.2-5)}$$

Q_k being the internal state partition function for particle k. Using the equations of change,[9,10] the differentiation of $f_k^{(0)}$ in equation (II.2-1) can be done to obtain an expression[3,11] for ψ_k:

$$\psi_k = 2[\underline{W}_k\underline{W}_k]^{(2)} : [\underline{\nabla}\underline{v}_0]^{(2)} + \left(\frac{2k_BT}{m_k}\right)^{1/2}\left[\left(W_k^2-\frac{5}{2}\right)+\frac{H_k'-\langle H_k'\rangle_k}{k_BT}\right]\underline{W}_k \cdot \underline{\nabla}\, \ell n\, T$$

$$+ \left(\frac{2k_BT}{m_k}\right)^{1/2}\frac{n}{n_k}\,\underline{W}_k \cdot \underline{d}_k + \frac{c_t}{c_v}\left[\left(\frac{2}{3}W_k^2-1\right) - \frac{H_k'-\langle H_k'\rangle_k}{c_{int}T}\right](\underline{\nabla}\cdot\underline{v}_0)\ . \tag{II.2-6}$$

In the above, the bracket notation, $[\ ]^{(a)}$, indicates a symmetric traceless tensor of rank a, c_v is the constant volume heat capacity per molecule, c_{int} is the internal heat capacity per molecule, $c_{int} = c_v - \frac{3}{2}k_B$, and, in the absence of external forces,[3] ($f^{(0)}$ has not been allowed to depend on external forces)

$$\underline{d}_k = \underline{\nabla}\left(\frac{n_k}{n}\right) + \left[\frac{n_k}{n} - \frac{n_k m_k}{\rho}\right]\underline{\nabla}\, \ell n\, p\ , \tag{II.2-7}$$

with

$$\sum_k \underline{d}_k = 0\ . \tag{II.2-8}$$

The perturbation, ϕ_k, is then expanded in gradients of the macroscopic variables describing the system:

$$\phi_k = -\underline{A}_k \cdot \underline{\nabla}\, \ell n\, T - \underline{\underline{B}}_k : [\underline{\nabla}\underline{v}_0]^{(2)} + n\sum_{\ell=1}^{2} \underline{C}_{k\ell}\cdot\underline{d}_\ell - D_k\underline{\nabla}\cdot\underline{v}_0\ , \tag{II.2.9}$$

in which $\underline{A}_k$, $\underline{\underline{B}}_k$, $\underline{C}_{k\ell}$, and D_k are functions of the local velocity, composition, and temperature.[3] Since the gradients in equations (II.2-6) and (II.2-9) are independent, the integral equations separate:

$$2(\underline{W}_k\underline{W}_k - \frac{1}{3}W_k^2 \underline{\underline{U}}) = iL_k\underline{\underline{B}}_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}\underline{\underline{B}}_k + \mathcal{R}''_{k\ell}\underline{\underline{B}}_\ell) , \tag{II.2-10}$$

where $\underline{\underline{U}}$ is the second rank unit tensor,

$$\left(\frac{2k_BT}{m_k}\right)^{1/2} \left[(W_k^2 - \frac{5}{2}) + \frac{H'_k - \langle H'_k\rangle_k}{k_BT}\right]\underline{W}_k = iL_k\underline{A}_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}\underline{A}_k + \mathcal{R}''_{k\ell}\underline{A}_\ell) , \tag{II.2-11}$$

$$\frac{c_{int}}{c_v}\left[(\frac{2}{3}W_k^2 - 1) - \frac{H'_k - \langle H'_k\rangle_k}{c_{int}T}\right] = iL_kD_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}D_k + \mathcal{R}''_{k\ell}D_\ell) , \tag{II.2-12}$$

and

$$\left(\frac{2k_BT}{m_k}\right)^{1/2} \frac{1}{n_k}\underline{W}_k(\delta_{kj} - \delta_{ki}) = iL_k(\underline{C}_{ki} - \underline{C}_{kj}) + \sum_{\ell=1}^{2} [\mathcal{R}'_{k\ell}(\underline{C}_{ki} - \underline{C}_{kj}) + \mathcal{R}''_{k\ell}(\underline{C}_{\ell i} - \underline{C}_{\ell j})] , \tag{II.2-13}$$

The last equation is obtained by consideration of the condition on the $\underline{d}_k$ stated in (II.2-8).

Equation (II.2-10) requires that $\underline{\underline{B}}_k$ be a symmetric, traceless tensor. Thus, it automatically satisfies all three of the auxiliary conditions[8] expressed in equations (II.2-4). The $\underline{A}_k$ and $\underline{C}_{k\ell}$ automatically satisfy (II.2-4a) and (II.2-4c), however, (II.2-4b) yields the two auxiliary conditions:

$$0 = \sum_k \sqrt{m_k}\, Tr_k \int f_k^{(0)} (\underline{A}_k \cdot \underline{W}_k)\, d\underline{p}_k \qquad (II.2\text{-}14)$$

and

$$0 = \sum_k \sqrt{m_k}\, Tr_k \int f_k^{(0)} ([\underline{C}_{ki} - \underline{C}_{kj}] \cdot \underline{W}_k)\, d\underline{p}_k \,. \qquad (II.2\text{-}15)$$

The D_k on the other hand, satisfy (II.2-4b) automatically, while (II.2-4a) and (II.2-4c) provide the remaining two auxiliary conditions:

$$0 = Tr_k \int f_k^{(0)} D_k\, d\underline{p}_k \qquad (II.2\text{-}16a)$$

and

$$0 = \sum_k Tr_k \int f_k^{(0)} D_k \left[W_k + \frac{H_k'}{k_B T}\right] d\underline{p}_k \,. \qquad (II.2\text{-}16b)$$

The integral equations, (II.2-10) through (II.2-13), along with the auxiliary conditions stated in equations (II.2-14) through (II.2-16), may now be solved for the $\underline{A}_k$, $\underline{\underline{B}}_k$, $\underline{C}_{k\ell}$, and D_k. It is useful at this point, however, to obtain tensor equations for the transport coefficients in terms of these quantities. This is done in the following section.

II.3 Transport Properties of a Binary Mixture

In this section, the perturbation operator of section II.2 is used to obtain expressions for the pressure tensor, $\underline{\underline{P}}$, the diffusion velocity $\langle \underline{V}_k \rangle_{AV}$, the energy flux, $\underline{q}$, and the anisotropic, (symmetric, traceless) part of the dielectric tensor, $[\underline{\underline{\epsilon}}]^{(2)}$, in terms of the $\underline{A}_k$, $\underline{\underline{B}}_k$, $\underline{C}_{k\ell}$, and D_k . Comparison with phenomenological expressions for $\underline{\underline{P}}$, $\langle \underline{V}_k \rangle_{AV}$, $\underline{q}$, and $[\underline{\underline{\epsilon}}]^{(2)}$ in terms of the experimentally measureable transport coefficients yields expressions for the transport properties in terms of the $\underline{A}_k$, $\underline{\underline{B}}_k$, $\underline{C}_{k\ell}$, and D_k .

The pressure tensor is given by the following phenomenological relation: [3]

$$\underline{\underline{P}} = p\underline{\underline{U}} - 2\underline{\underline{\eta}} : [\underline{\nabla}\underline{v}_0]^{(2)} - \underline{\underline{\kappa}}(\underline{\nabla}\cdot\underline{v}_0) , \qquad (II.3\text{-}1)$$

in which p is the scalar pressure, $[\underline{\nabla}\underline{v}_0]^{(2)}$ is the rate of shear tensor (symmetric and traceless), $\underline{\underline{\eta}}$ is the shear viscosity tensor (of rank, 4), and $\underline{\underline{\kappa}}$ is the bulk viscosity tensor (of rank, 2). In terms of the distribution function-density operator, [9] f_k ,

$$\begin{aligned} \underline{\underline{P}} &= 2k_BT \sum_k \mathrm{Tr}_k \int f_k \underline{W}_k \underline{W}_k \, d\underline{p}_k \\ &= 2k_BT \sum_k \mathrm{Tr}_k \int f_k^{(0)} (1+\phi_k) \underline{W}_k \underline{W}_k \, d\underline{p}_k . \end{aligned} \qquad (II.3\text{-}2)$$

Neglecting the terms involving temperature and concentration gradients,

$$\underline{\underline{P}} = 2k_BT \sum_k \{\mathrm{Tr}_k \int f_k^{(0)} \underline{W}_k\underline{W}_k d\underline{p}_k - \mathrm{Tr}_k \int f_k^{(0)} \underline{W}_k\underline{W}_k\underline{\underline{B}}_k : \underline{\nabla}\underline{v}_0 d\underline{p}_k \tag{II.3-3}$$

$$- \mathrm{Tr}_k \int f_k^{(0)} \underline{W}_k\underline{W}_k D_k \underline{\nabla}\cdot\underline{v}_0 d\underline{p}_k\} .$$

In the above, and in the equations to follow, the integration over $\underline{p}_k$ can equally well be taken to be an integration over particle momentum or peculiar momentum.

The following identifications can now be made: [9]

$$\sum_k \mathrm{Tr}_k \int F(W_k)\underline{W}_k\underline{W}_k d\underline{p}_k = \frac{1}{3}\underline{\underline{U}} \sum_k \mathrm{Tr}_k \int F(W_k) W_k^2 d\underline{p}_k , \tag{II.3-4}$$

yielding
$$p = \frac{2k_BT}{3} \sum_k \mathrm{Tr}_k \int f_k^{(0)} W_k^2 d\underline{p}_k = nk_BT ; \tag{II.3-5}$$

$$\underline{\underline{\eta}} = k_BT \sum_k \mathrm{Tr}_k \int f_k^{(0)} \underline{W}_k\underline{W}_k\underline{\underline{B}}_k d\underline{p}_k , \tag{II.3-6}$$

since $\underline{\underline{B}}_k$ is symmetric and traceless; and

$$\underline{\underline{\kappa}} = 2k_{BT} \sum_k \mathrm{Tr}_k \int f_k^{(0)} \underline{W}_k\underline{W}_k D_k d\underline{p}_k . \tag{II.3-7}$$

Similarly, a phenomenological relation involving the diffusion velocity is given by the expression: [3]

$$n_k m_k \langle \underline{V}_k \rangle_{AV} = \frac{n^2 m_k}{\rho} \sum_{\ell} m_{\ell} \underline{\underline{D}}_{k\ell} \cdot \underline{d}_{\ell} - \underline{\underline{D}}_k^T \cdot \underline{\nabla} \ln T \, , \qquad \text{(II.3-8)}$$

in which $\underline{\underline{D}}_{k\ell}$ and $\underline{\underline{D}}_k^T$ are the multicomponent diffusion and thermal diffusion tensors, respectively. In terms of the distribution function-density operator, [3,9]

$$\langle \underline{V}_k \rangle_{AV} = \frac{1}{n_k} Tr_k \int f_k \underline{V}_k d\underline{p}_k \, , \qquad \text{(II.3-9)}$$

and consequently, neglecting terms involving $\underline{\nabla}\underline{v}_0$ and $\underline{\nabla} \cdot \underline{v}_0$,

$$\begin{aligned} n_k m_k \langle \underline{V}_k \rangle_{AV} = & -m_k \, Tr_k \int f_k^{(0)} \underline{V}_k \underline{A}_k \cdot \underline{\nabla} \ln T \, d\underline{p}_k \\ & + m_k n \sum_{\ell} Tr_k \int f_k^{(0)} \underline{V}_k \underline{C}_{k\ell} \cdot \underline{d}_{\ell} \, d\underline{p}_k \, , \end{aligned} \qquad \text{(II.3-10)}$$

since

$$Tr_k \int f_k^{(0)} \underline{V}_k \, d\underline{p}_k = 0 \qquad \text{(II.3-11)}$$

In this case, the following identifications can be made immediately: [11]

$$\underline{\underline{D}}_{k\ell} = \frac{\rho}{n m_{\ell}} Tr_k \int f_k^{(0)} \underline{V}_k \underline{C}_{k\ell} \, d\underline{p}_k \qquad \text{(II.3-12)}$$

and

$$\underline{\underline{D}}_k^T = m_k \, Tr_k \int f_k^{(0)} \underline{V}_k \underline{A}_k \, d\underline{p}_k \, . \qquad \text{(II.3-13)}$$

The phenomenological expression for the energy flux [3,9] is

$$\underline{q} = k_B T \sum_k \left(\frac{5}{2} + \frac{\langle H_k' \rangle_k}{k_B T}\right) n_k \langle \underline{V}_k \rangle_{AV} - \underline{\underline{\lambda}}_0 \cdot \underline{\nabla} T$$
$$- n k_B T \sum_k \frac{1}{n_k m_k} \underline{\underline{D}}_k^T \cdot \underline{d}_k \, , \qquad \text{(II.3-14)}$$

in which $\underline{\underline{\lambda}}_0$ is the thermal conductivity tensor for a gas mixture of uniform composition, that is, $\underline{\underline{\lambda}}_0$ is the thermal conductivity tensor in the limit that no thermal diffusion has occurred. If equation (II.3-8) is solved for the $\underline{d}_\ell$ in terms of $\langle \underline{V}_k \rangle_{AV}$ and $\underline{\nabla} T$, and the result inserted in (II.3-14), the new coefficient of $\underline{\nabla} T$ is $-\underline{\underline{\lambda}}_\infty$, the thermal conductivity tensor which is ordinarily measured.

In terms of f_k, the energy flux, neglecting terms involving $\underline{\nabla}\underline{v}_0$ and $\underline{\nabla} \cdot \underline{v}_0$, is given by: [3,8,9]

$$\underset{\sim}{q} = \sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \mathrm{Tr}_k \int f_k(k_BTW_k^2 + H_k')\underset{\sim}{W}_k \, d\underset{\sim}{p}_k$$

$$= \sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \{-\mathrm{Tr}_k \int f_k^{(0)}(k_BTW_k^2 + H_k')\underset{\sim}{W}_k\underset{\sim}{A}_k \cdot \underset{\sim}{\nabla} \ln T \, d\underset{\sim}{p}_k$$

$$+ n \sum_\ell \mathrm{Tr}_k \int f_k^{(0)}(k_BTW_k^2 + H_k')\underset{\sim}{W}_k\underset{\sim}{C}_{k\ell} \cdot \underset{\sim}{d}_\ell \, d\underset{\sim}{p}_k\} \, , \tag{II.3-15}$$

since

$$\int f_k^{(0)}(k_BTW_k^2 + H_k')\underset{\sim}{W}_k \, d\underset{\sim}{p}_k = 0 \, . \tag{II.3-16}$$

Now, using (II.3-10),

$$k_BT \sum_k \left(\frac{5}{2} + \frac{\langle H_k' \rangle_k}{k_BT}\right) n_k \langle \underset{\sim}{V}_k \rangle_{AV} = -k_BT \sum_k \left(\frac{5}{2} + \frac{\langle H_k' \rangle_k}{k_BT}\right) \tag{II.3-17}$$

$$\times \{\mathrm{Tr}_k \int f_k^{(0)}\underset{\sim}{V}_k\underset{\sim}{A}_k \cdot \underset{\sim}{\nabla} \ln T \, d\underset{\sim}{p}_k - \sum_\ell n \, \mathrm{Tr}_k \int f_k^{(0)}\underset{\sim}{V}_k\underset{\sim}{C}_{k\ell} \cdot \underset{\sim}{d}_\ell \, d\underset{\sim}{p}_k\} \, ,$$

allowing (II.3-15) to be rewritten:

$$\underset{\sim}{q} = k_BT \sum_k \left(\frac{5}{2} + \frac{\langle H_k' \rangle_k}{k_BT}\right) n_k \langle \underset{\sim}{V}_k \rangle_{AV} \tag{II.3-18}$$

$$- k_BT \sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \{\mathrm{Tr}_k \int f_k^{(0)}\left(W_k^2 + \frac{H_k'}{k_BT} - \frac{5}{2} - \frac{\langle H_k' \rangle_k}{k_BT}\right)$$

$$\times \underset{\sim}{W}_k\underset{\sim}{A}_k \cdot \underset{\sim}{\nabla} \ln T \, d\underset{\sim}{p}_k - n \sum_\ell \mathrm{Tr}_k \int f_k^{(0)}\left(W_k^2 + \frac{H_k'}{k_BT} - \frac{5}{2} - \frac{\langle H_k' \rangle_k}{k_BT}\right)\underset{\sim}{W}_k\underset{\sim}{C}_{k\ell} \cdot \underset{\sim}{d}_\ell \, d\underset{\sim}{p}_k\} \, .$$

By using equations (II.2-11) and (II.2-13) along with the symmetry properties[6,8,12] of $\mathcal{R}'_{k\ell}$, $\mathcal{R}''_{k\ell}$, and L_k , it is possible to show that (see Appendix II.A)

$$\sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \sum_\ell \mathrm{Tr}_k \int f_k^{(0)} \left(W_k^2 + \frac{H'_k}{k_BT} - \frac{5}{2} - \frac{\langle H'_k \rangle_k}{k_BT}\right) \underline{W}_k \underline{C}_{k\ell} \cdot \underline{d}_\ell \, d\underline{p}_k$$

$$= - \sum_\ell \frac{1}{m_\ell n_\ell} \underline{\underline{D}}_\ell^T \cdot \underline{d}_\ell \, , \tag{II.3-19}$$

yielding

$$\underline{q} = k_BT \sum_k \left(\frac{5}{2} + \frac{\langle H'_k \rangle_k}{k_BT}\right) n_k \langle \underline{V}_k \rangle_{AV}$$

$$- k_BT \sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \mathrm{Tr}_k \int f_k^{(0)} \left(W_k^2 + \frac{H'_k}{k_BT} - \frac{5}{2} - \frac{\langle H'_k \rangle_k}{k_BT}\right) \underline{W}_k \underline{A}_k \cdot \underline{\nabla} \ln T \, d\underline{p}_k$$

$$- nk_BT \sum_\ell \frac{1}{m_\ell n_\ell} \underline{\underline{D}}_\ell^T \cdot \underline{d}_\ell \, , \tag{II.3-20}$$

from which the identification can be made that

$$\underline{\underline{\lambda}}_0 = k_B \sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \mathrm{Tr}_k \int f_k^{(0)} \left(W_k^2 - \frac{5}{2} + \frac{H'_k - \langle H'_k \rangle_k}{k_BT}\right) \underline{W}_k \underline{A}_k \, d\underline{p}_k \, . \tag{II.3-21}$$

Finally, if only gradients in $\underline{v}_0$ need be considered, the symmetric, traceless part of the dielectric tensor is given by the phenomenological expression:[13]

$$[\underline{\underline{\epsilon}}]^{(2)} = -2\underline{\underline{\beta}} : [\nabla \underline{v}_0]^{(2)} \ , \qquad \text{(II.3-22)}$$

in which $\underline{\underline{\beta}}$ is the flow birefringence tensor (of rank, 4). In terms of the distribution function-density operator,[13]

$$[\underline{\underline{\epsilon}}]^{(2)} = -2\pi\sqrt{\frac{2}{15}} \sum_k n_k (\alpha_{||} - \alpha_{\perp})_k \mathrm{Tr}_k \int d\underline{p}_k f_k \{\sqrt{\frac{15}{2}} [\underline{J}_k^2(\underline{J}_k^2 - \frac{3}{4})]^{-1/2} [\underline{J}_k \underline{J}_k]^{(2)}\}^{+}$$

$$= 2\pi \sum_k n_k (\alpha_{||} - \alpha_{\perp})_k \mathrm{Tr}_k \int d\underline{p}_k f_k^{(0)} \{\underline{J}_k^2(\underline{J}_k^2 - \frac{3}{4})]^{-1/2} [\underline{J}_k \underline{J}_k]^{(2)}\}^{+} \underline{\underline{B}}_k : \nabla \underline{v}_0 \ ,$$

(II.3-23)

in which $\alpha_{||}$ and $\alpha_{\perp}$ are the electric polarizabilities of a molecule parallel and perpendicular to the symmetry axis of the molecule, respectively, and in which the second rank tensor, $\{\sqrt{\frac{15}{2}}[\underline{J}_k^2(\underline{J}_k^2 - \frac{3}{4})]^{-1/2}[\underline{J}_k \underline{J}_k]^{(2)}\}$, characterizes the angular momentum polarization[14] of the molecules of species k. Again, the identification is immediate:

$$\underline{\underline{\beta}} = -\pi \sum_k n_k (\alpha_{||} - \alpha_{\perp})_k \mathrm{Tr}_k \int f_k^{(0)} \{[\underline{J}_k^2(\underline{J}_k^2 - \frac{3}{4})]^{-1/2} [\underline{J}_k \underline{J}_k]^{(2)}\}^{+} \underline{\underline{B}}_k \, d\underline{p}_k \ .$$

(II.3-24)

Using the perturbation of section II.2, expressions have been obtained for the shear viscosity tensor, $\underline{\underline{\eta}}$, the bulk viscosity tensor, $\underline{\underline{\kappa}}$, the multicomponent diffusion tensor, $\underline{\underline{D}}_{k\ell}$, the thermal diffusion tensor, $\underline{\underline{D}}_k^T$, the uniform composition thermal conductivity tensor, $\underline{\underline{\lambda}}_0$, and the flow birefringence tensor, $\underline{\underline{\beta}}$. In the following section, scalar equations are obtained for the above quantities, yielding expressions more useful for computational purposes.

II.4 Scalar Equations for the Transport Properties

Equations (II.2-10) through (II.2-13) can be written in terms of tensors in the Wang Chang-Uhlenbeck basis. Expansion of the unknown tensors of the perturbation operator appearing in these equations over a total polarization basis leads to a partial uncoupling due to the conservation of polarization.[8] This yields the desired scalar equations for the transport properties.

In Ref. 12, the Wang Chang-Uhlenbeck basis elements are defined:

$$\underline{\underline{B}}_{k;pqst} \equiv \underline{\underline{L}}^{ps}(\underline{W}_k)[\underline{J}_k]^{(q)} R_t^{(q)}(H_k/k_B T) \ , \qquad \text{(II.4-1)}$$

the $\underline{\underline{L}}^{ps}(\underline{W}_k)$ being velocity tensors composed of a product of an irreducible Cartesian tensor, $[\underline{W}]^{(p)}$, of weight p, and an appropriately normalized[7] associated Laguerre function, $L_s^{(p+1/2)}(W_k^2)$. The left hand sides of equations (II.2-10) through (II.2-13) are expressible in terms of the $\underline{\underline{B}}_{k;pqst}$ elements just defined. (II.2-10) through (II.2-13) can then be written

$$iL_k\underline{\underline{B}}_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}\underline{\underline{B}}_k + \mathcal{R}''_{k\ell}\underline{\underline{B}}_\ell) = 2(\underline{W}_k\underline{W}_k - \tfrac{1}{3}W_k^2\underline{\underline{U}})$$

$$= \sqrt{2}\,\underline{\underline{L}}^{20}(\underline{W}_k) \qquad \text{(II.4-2)}$$

$$= \sqrt{2}\,\underline{\underline{B}}_{k;2000} ,$$

$$iL_k\underline{A}_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}\underline{A}_k + \mathcal{R}''_{k\ell}\underline{A}_\ell) = \left(\frac{2k_BT}{m_k}\right)^{1/2}\left[\left(W_k^2 - \frac{5}{2}\right) + \frac{H'_k - \langle H'_k\rangle_k}{k_BT}\right]\underline{W}_k$$

$$= \left(\frac{2k_BT}{m_k}\right)^{1/2}\left[-\sqrt{\frac{5}{4}}\,\underline{\underline{L}}^{11}(\underline{W}_k) + \frac{1}{\sqrt{2}}\,\underline{\underline{L}}^{10}(\underline{W}_k)\sqrt{\frac{c^k_{int}}{k_B}}\,R_1^{(0)}(H_k/k_BT)\right]$$

$$= \left(\frac{k_BT}{m_k}\right)^{1/2}\left[-\sqrt{\frac{5}{2}}\,\underline{\underline{B}}_{k;1010} + \sqrt{\frac{c^k_{int}}{k_B}}\,\underline{\underline{B}}_{k;1001}\right] , \qquad \text{(II.4-3)}$$

$$iL_kD_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell}D_k + \mathcal{R}''_{k\ell}D_\ell) = \frac{c_{int}}{c_v}\left[\left(\frac{2}{3}W_k^2 - 1\right) - \frac{H'_k - \langle H'_k\rangle_k}{T}\right]$$

$$= \frac{c_{int}}{c_v}\left[-\sqrt{\frac{2}{3}}\,\underline{\underline{L}}^{01}(\underline{W}_k) - \frac{k_B}{c_{int}}\sqrt{\frac{c^k_{int}}{k_B}}\,R_1^{(0)}(H_k/k_BT)\right]$$

$$= \frac{c_{int}}{c_v}\left[-\sqrt{\frac{2}{3}}\,\underline{\underline{B}}_{k;0010} - \frac{k_B}{c_{int}}\sqrt{\frac{c^k_{int}}{k_B}}\,\underline{\underline{B}}_{k;0001}\right] , \qquad \text{(II.4-4)}$$

and

$$i L_k(\underline{C}_{ki}-\underline{C}_{kj}) + \sum_{\ell=1}^{2} [(\delta\Omega'_{k\ell}(\underline{C}_{ki}-\underline{C}_{kj})+\delta\Omega''_{k\ell}(\underline{C}_{\ell i}-\underline{C}_{\ell j})]$$

$$= \left(\frac{2k_BT}{m_k}\right)^{1/2}\frac{1}{n_k}\underline{W}_k(\delta_{kj}-\delta_{ki})$$

$$= \left(\frac{2k_BT}{m_k}\right)^{1/2}\frac{1}{\sqrt{2}\,n_k}\underline{\underline{L}}^{10}(\underline{W}_k)(\delta_{kj}-\delta_{ki}) \qquad \text{(II.4-5)}$$

$$= \left(\frac{k_BT}{m_k}\right)^{1/2}\frac{1}{n_k}\underline{\underline{B}}_{k;1000}(\delta_{kj}-\delta_{ki}) \ .$$

The transformation of (II.4-2), (II-4-3), and (II.4-5) to scalar equations is accomplished by writing them in terms of their spherical components. As in Hunter's treatment of a single component system,[8] the spherical basis chosen is that of Chen, Moraal, and Snider.[12] Their basis tensors, $\underline{\underline{e}}^{pm}$, transform under rotation according to the irreducible representation of the rotation group. Furthermore,

$$\underline{\underline{e}}^{p}_{m'} \odot^{p} \underline{\underline{e}}^{pm} = \delta_{m,m'} \qquad \text{(II.4-6)}$$

where

$$\underline{\underline{e}}^{p}_{m'} = (\underline{\underline{e}}^{pm'})^{*} \ ,$$

and

$$\sum_{m} \underline{\underline{e}}^{p}_{m}\underline{\underline{e}}^{pm} = \underline{\underline{E}}^{(p)} \ , \qquad \text{(II.4-7)}$$

where $\underline{\underline{E}}^{(p)}$ is the projection operator onto the space of p-th rank symmetric traceless tensors. Consequently, the $\underline{\underline{e}}^{pm}$ are orthonormal and complete.

The $\underline{\underline{B}}_k$ appearing on the LHS of (II.4-2) are symmetric traceless tensors of rank 2, and consequently, their spherical components are obtained by dotting them with $\underline{\underline{e}}^{2m}$:

$$B_k^m = \underline{\underline{e}}^{2m} \odot^2 \underline{\underline{B}}_k . \qquad \text{(II.4-8)}$$

The $\underline{A}_k$ and $\underline{C}_{ki}$ of equations (II.4-3) and (II.4-5) are of rank 1, and so their spherical components are obtained by dotting them with $\underline{e}^{1m}$:

$$A_k^m = \underline{e}^{1m} \odot \underline{A}_k \qquad \text{(II.4-9a)}$$

and

$$C_{ki}^m = \underline{e}^{1m} \odot \underline{C}_{ki} . \qquad \text{(II.4-9b)}$$

Note that (II.4-8) and (II.4-9a) are simply component versions of H-44 and H-52.

Using the above and the fact that the spherical components of the $\underline{\underline{B}}_{k;post}$ are given by [8]

$$B_{k;post}^{mo} = \underline{\underline{e}}^{pm} \odot^p \underline{\underline{B}}_{k;post} , \qquad \text{(II.4-10)}$$

it is possible to obtain scalar equations from (II.4-2), (II.4-3), and (II.4-5) by dotting (II.4-2) with $\underline{\underline{e}}^{2m}$, and (II.4-3) and (II.4-5) with $\underline{e}^{1m}$. In addition, noting that $\underline{\underline{B}}_{k;oost}$ is a zeroth rank tensor, i.e.,

$$\underline{\underline{B}}_{k;oost} = B_{k;oost} , \qquad \text{(II.4-11)}$$

(II.4-2) through (II.4-5) can be written in scalar form:

$$\sqrt{2}\, B^{mo}_{k;2000} = iL_k B^m_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell} B^m_k + \mathcal{R}''_{k\ell} B^m_\ell) , \qquad \text{(II.4-12)}$$

$$\left(\frac{k_B T}{m_k}\right)^{1/2} \left[\sqrt{\frac{c^k_{int}}{k_B}}\, B^{mo}_{k;1001} - \sqrt{\frac{5}{2}}\, B^{mo}_{k;1010}\right] = iL_k A^m_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell} A^m_k + \mathcal{R}''_{k\ell} A^m_\ell) , \qquad \text{(II.4-13)}$$

$$-\frac{c_{int}}{c_v}\left[\sqrt{\frac{2}{3}}\, B_{k;0010} + \frac{\sqrt{k_B c^k_{int}}}{c_{int}}\, B_{k;0001}\right] = iL_k D_k + \sum_{\ell=1}^{2} (\mathcal{R}'_{k\ell} D_k + \mathcal{R}''_{k\ell} D_\ell) , \qquad \text{(II.4-14)}$$

and

$$\left(\frac{k_B T}{m_k}\right)^{1/2} \frac{1}{n_k}\, B^{mo}_{k;1000}\, (\delta_{kj} - \delta_{ki}) = iL_k (C^m_{ki} - C^m_{kj}) + \sum_{\ell=1}^{2} [\mathcal{R}'_{k\ell} (C^m_{ki} - C^m_{kj}) + \mathcal{R}''_{k\ell} (C^m_{\ell i} - C^m_{\ell j})] . \qquad \text{(II.4-15)}$$

The spherical components of the Wang Chang-Uhlenbeck basis operators are given by

$$B^{\mu\nu}_{k;pqst} = \underline{\underline{e}}^{p\mu} \odot^{p} \underline{\underline{B}}_{k;pqst} \odot^{q} \underline{\underline{e}}^{q\nu} , \qquad \text{(II.4-16a)}$$

which in turn yield the spherical components of the total polarization basis: [8]

$$B^{(a)\alpha}_{k;pqst} = (-1)^{a+\alpha} \sum_{\mu\nu} \begin{pmatrix} p & q & a \\ \mu & \nu & -\alpha \end{pmatrix} B^{\mu\nu}_{k;pqst} . \qquad \text{(II.4-16b)}$$

The components of the perturbation operator are now expanded over the total polarization basis:

$$B^{m}_{\ell} = \sum_{pqsta} B^{pqst}_{(a)m;\ell} \, B^{(a)m}_{\ell;pqst} , \qquad \text{(II.4-17a)}$$

$$A^{m}_{\ell} = \sum_{pqsta} A^{pqst}_{(a)m;\ell} \, B^{(a)m}_{\ell;pqst} , \qquad \text{(II.4-17b)}$$

$$D_{\ell} = D^{0}_{\ell} = \sum_{pqsta} D^{pqst}_{(a)0;\ell} \, B^{(a)0}_{\ell;pqst} , \qquad \text{(II.4-17c)}$$

and

$$C^{m}_{\ell i} = \sum_{pqsta} C^{pqst}_{(a)m;\ell i} \, B^{(a)m}_{\ell;pqst} , \qquad \text{(II.4-17d)}$$

in which the $B^{(a)m}_{\ell;pqst}$ are the basis elements, and $B^{pqst}_{(a)m;\ell}$, $A^{pqst}_{(a)m;\ell}$, $D^{pqst}_{(a)0;\ell}$, and $C^{pqst}_{(a)m;\ell i}$ are the unknown expansion coefficients.

Utilizing the above,

$$\sqrt{2}\, B^{(2)m}_{k;2000} = \sum_{\ell=1}^{2} \sum_{pqsta} \{[B^{pqst}_{(a)m;k}(\mathcal{R}'_{k\ell}+i\delta_{k\ell}L_k)B^{(a)m}_{k;pqst}]$$

$$+ [B^{pqst}_{(a)m;\ell}\,\mathcal{R}''_{k\ell}\,B^{(a)m}_{\ell;pqst}]\} \,, \qquad \text{(II.4-18)}$$

$$\left(\frac{k_B T}{m_k}\right)^{1/2}\left[\sqrt{\frac{c^k_{int}}{k_B}}\, B^{(1)m}_{k;1001} - \sqrt{\frac{5}{2}}\, B^{(1)m}_{k;1010}\right] \qquad \text{(II.4-19)}$$

$$= \sum_{\ell=1}^{2} \sum_{pqsta} \{[A^{pqst}_{(a)m;k}(\mathcal{R}'_{k\ell}+i\delta_{k\ell}L_k)B^{(a)m}_{k;pqst}] + [A^{pqst}_{(a)m;\ell}\,\mathcal{R}''_{k\ell}\,B^{(a)m}_{\ell;pqst}]\}$$

$$\frac{c_{int}}{c_v}\left[\sqrt{\frac{2}{3}}\,B_{k;0010} + \frac{\sqrt{k_B c^k_{int}}}{c_{int}}\, B_{k;0001}\right] \qquad \text{(II.4-20)}$$

$$= -\sum_{\ell=1}^{2} \sum_{pqsta} \{[D^{pqst}_{(a)0;k}(\mathcal{R}'_{k\ell}+i\delta_{k\ell}L_k)B^{(a)0}_{k;pqst}] + [D^{pqst}_{(a)0;\ell}\,\mathcal{R}''_{k\ell}\,B^{(a)0}_{\ell;pqst}]\} \,,$$

and

$$\left(\frac{k_B T}{m_k}\right)^{1/2} \frac{1}{n_k}\, B^{(1)m}_{k;1000}(\delta_{kj}-\delta_{ki})$$

$$= \sum_{\ell=1}^{2} \sum_{pqsta} \{[(C^{pqst}_{(a)m;ki} - C^{pqst}_{(a)m;kj})(\mathcal{R}'_{k\ell}+i\delta_{k\ell}L_k)B^{(a)m}_{k;pqst}] \qquad \text{(II.4-21)}$$

$$+ [(C^{pqst}_{(a)m;\ell i} - C^{pqst}_{(a)m;\ell j})\mathcal{R}''_{k\ell}\,B^{(a)m}_{\ell;pqst}]\} \,.$$

The basis elements, $B^{(a)\alpha}_{k;pqst}$, are normalized such that

$$\langle\langle B^{(a)\alpha}_{k;pqst} | B^{(a')\alpha'}_{k;p'q's't'} \rangle\rangle_k = \delta(a\alpha|a'\alpha')\delta(pqst|p'q's't') , \tag{II.4-22}$$

where the inner product for mixtures is defined [12] as

$$\langle\langle A_k | B_k \rangle\rangle_k \equiv \frac{1}{n_k} Tr_k \int d\underline{p}_k \, f^{(0)}_k \, A^{\dagger}_k B_k . \tag{II.4-23}$$

Multiplying equations (II.4-18) through (II.4-21) from the left by $B^{(a')m'+}_{k;p'q's't'}$ and taking the inner product, the following set of matrix equations is obtained:

$$\sqrt{2}\,\delta(p'q's't'a'|20002)$$

$$= \sum_{\ell=1}^{2} \sum_{pqsta} \{[B^{pqst}_{(a)m;k} \langle\langle B^{(a')m'}_{k;p'q's't'} | (\mathcal{R}'_{k\ell} + i\epsilon_{k\ell} L_k) | B^{(a)m}_{k;pqst} \rangle\rangle_k] \tag{II.4-24}$$

$$+ [B^{pqst}_{(a)m;\ell} \langle\langle B^{(a')m'}_{k;p'q's't'} | \mathcal{R}''_{k\ell} | B^{(a)m}_{\ell;pqst} \rangle\rangle_k]\} .$$

$$\left(\frac{k_B T}{m_k}\right)^{1/2} \left[\sqrt{\frac{c^k_{int}}{k_B}}\, \delta(p'q's't'a'|10011) - \sqrt{\frac{5}{2}}\, \delta(p'q's't'a'|10101) \right]$$

$$= \sum_{\ell=1}^{2} \sum_{pqsta} \{[A^{pqst}_{(a)m;k} \langle\langle B^{(a')m'}_{k;p'q's't'} | (\mathcal{R}'_{k\ell} + i\epsilon_{k\ell} L_k) | B^{(a)m}_{k;pqst} \rangle\rangle_k] \tag{II.4-25}$$

$$+ [A^{pqst}_{(a)m;\ell} \langle\langle B^{(a')m'}_{k;p'q's't'} | \mathcal{R}''_{k\ell} | B^{(a)m}_{k;pqst} \rangle\rangle_k]\} ,$$

$$\frac{c_{int}}{c_v}\left[\sqrt{\frac{2}{3}}\ \delta(p'q's't'a'|00100) + \frac{\sqrt{k_B c^k_{int}}}{c_{int}}\ \delta(p'q's't'a'|00010)\right]$$

$$= -\sum_{\ell=1}^{2}\sum_{pqsta}\{[D^{pqst}_{(a)0;k} \ll B^{(a')m'}_{k;p'q's't'}|(\mathcal{R}'_{k\ell}+i\delta_{k\ell}L_k)|B^{(a)0}_{k;pqst}\gg_k]$$

$$+ [D^{pqst}_{(a)0;\ell} \ll B^{(a')m'}_{k;p'q's't'}|\mathcal{R}''_{k\ell}|B^{(a)0}_{\ell;pqst}\gg_k]\} \ , \tag{II.4-26}$$

and

$$\left(\frac{k_B T}{m_k}\right)^{1/2}\frac{1}{n_k}\ \delta(p'q's't'a'|10001)(\delta_{kj}-\delta_{ki})$$

$$= \sum_{\ell=1}^{2}\sum_{pqsta}\{[(C^{pqst}_{(a)m;ki} - C^{pqst}_{(a)m;kj})$$

$$\times \ll B^{(a')m'}_{k;p'q's't'}|(\mathcal{R}''_{k\ell}+i\delta_{k\ell}L_k)|B^{(a)m}_{k;pqst}\gg_k] \tag{II.4-27}$$

$$+ [(C^{pqst}_{(a)m;\ell i} - C^{pqst}_{(a)m;\ell j}) \ll B^{(a')m'}_{k;p'q's't'}|\mathcal{R}''_{k\ell}|B^{(a)m}_{\ell;pqst}\gg_k]\} \ .$$

The fact that $\mathcal{R}'_{k\ell}$ and $\mathcal{R}''_{k\ell}$ are invariant under all rotations,[8] and consequently conserve both total polarization indices, allows their matrix elements to be written

$$\ll B^{(a')\alpha'}_{k;p'q's't'}|\mathcal{R}'_{k\ell}|B^{(a)\alpha}_{k;pqst}\gg_k = \delta(a'\alpha'|a\alpha) \ll B^{(a)\alpha}_{k;p'q's't'}|\mathcal{R}'_{k\ell}|B^{(a)\alpha}_{k;pqst}\gg_k \ , \tag{II.4-28a}$$

and

$$\ll B^{(a')\alpha'}_{k;p'q's't'}|\mathcal{R}''_{k\ell}|B^{(a)\alpha}_{k;pqst}\gg_k = \delta(a'\alpha'|a\alpha)\ll B^{(a)\alpha}_{k;p'q's't'}|\mathcal{R}''_{k\ell}|B^{(a)\alpha}_{k;pqst}\gg_k .$$

(II.4-28b)

It is convenient to define two scalar quantities as the matrix elements appearing on the RHS of (II.4-28a) and (II.4-28b):

$$S'\begin{Bmatrix} p' & q' & s' & t' \\ p & q & s & t \end{Bmatrix}^{(a)}_{k\ell} \equiv \ll B^{(a)\alpha}_{k;p'q's't'}|\mathcal{R}''_{k\ell}|B^{(a)\alpha}_{k;pqst}\gg_k ,$$

(II.4-29a)

and

$$S''\begin{Bmatrix} p' & q' & s' & t' \\ p & q & s & t \end{Bmatrix}^{(a)}_{k\ell} \equiv \ll B^{(a)\alpha}_{k;p'q's't'}|\mathcal{R}''_{k\ell}|B^{(a)\alpha}_{\ell;pqst}\gg_\ell .$$

(II.4-29b)

L_k , on the other hand, is invariant only to rotations about the field direction.[8] Consequently, it conserves only the α index, and explicitly,

$$\ll B^{(a')\alpha'}_{k;p'q's't'}|L_k|B^{(a)\alpha}_{k;pqst}\gg_k = (\omega_L)_k\ \delta(p'q's't'\alpha'|pqst\alpha)L^{(\alpha)}_{pq}(a'a) ,$$

(II.4-30a)

where

$$L^{(\alpha)}_{pq} = (-1)^{a+a'+\alpha}(-1)^{p+q+1}\sqrt{(2a+1)(2a'+1)}\sqrt{q(q+1)(2q+1)}\begin{pmatrix} 1 & a & a' \\ 0 & \alpha & -\alpha \end{pmatrix}\begin{Bmatrix} 1 & a & a' \\ p & q & q \end{Bmatrix} .$$

(II.4-30b)

Using the above, equations (II.4-24) through (II.4-27) can be rewritten:

$$\sqrt{2}\,\delta(pqsta|20002) = \sum_{\ell=1}^{2} \sum_{p'q's't'a'} \{B^{p'q's't'}_{(a')m;k}[\delta_{aa'}S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell}]$$

$$+ B^{p'q's't'}_{(a')m;\ell}[\delta_{aa'}S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell} + i\delta_{k\ell}(\omega_L)_k\delta(p'q's't'|pqst)L^{(m)}_{pq}(aa')]\},$$

(II.4-31)

$$\left(\frac{k_BT}{m_k}\right)^{1/2}\left[\sqrt{\frac{c^k_{int}}{k_B}}\,\delta(pqsta|10011) - \sqrt{\frac{5}{2}}\,\delta(pqsta|10101)\right]$$

$$= \sum_{\ell=1}^{2} \sum_{p'q's't'a'} \{A^{p'q's't'}_{(a')m;k}[\delta_{aa'}S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell}]$$

$$+ A^{p'q's't'}_{(a')m;\ell}[\delta_{aa'}S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell} + i\delta_{k\ell}(\omega_L)_k\delta(p'q's't'|pqst)L^{(m)}_{pq}(aa')]\},$$

(II.4-32)

$$\frac{c_{int}}{c_v}\left[\sqrt{\frac{2}{3}}\,\delta(pqsta|00100) + \frac{\sqrt{k_Bc^k_{int}}}{c_{int}}\,\delta(pqsta|00010)\right]$$

$$= \sum_{\ell=1}^{2} \sum_{p'q's't'a'} \{D^{p'q's't'}_{(a')0;k}[\delta_{aa'}S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell}]$$

$$+ D^{p'q's't'}_{(a')0;\ell}[\delta_{aa'}S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell} + i\delta_{k\ell}(\omega_L)_k\delta(p'q's't'|pqst)L^{(0)}_{pq}(aa')]\},$$

(II.4-33)

and

$$\left(\frac{k_B T}{m_k}\right)^{1/2}\frac{1}{n_k}\,\delta(pqsta|10001)(\delta_{kj}-\delta_{ki})$$

$$= \sum_{\ell=1}^{2}\sum_{p'q's't'a'}\{(C^{p'q's't'}_{(a')m;ki} - C^{p'q's't'}_{(a')m;kj})[\delta_{aa'}S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t'\end{Bmatrix}^{(a)}_{k\ell}]$$

$$+ (C^{p'q's't'}_{(a')m;\ell i} - C^{p'q's't'}_{(a')m;\ell j})[\delta_{aa'}S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t'\end{Bmatrix}^{(a)}_{k\ell} + i\delta_{k\ell}(\omega_L)_k\,\delta(p'q's't'|pqst)L^{(m)}_{pq}(aa')]\} .$$

(II.4-34)

The above set of matrix equations can be solved to obtain the expansion coefficients, $B^{p'q's't'}_{(a')m;k}$, $A^{p'q's't'}_{(a')m;k}$, $D^{p'q's't'}_{(a')0;k}$, and $C^{p'q's't'}_{(a')m;ki}$, subject to the following auxiliary conditions:[8]

$$0 = \sum_k n_k\sqrt{m_k}\,A^{1000}_{1m;k} , \qquad \text{(II.4-35)}$$

$$0 = \sum_k n_k\sqrt{m_k}\,(C^{1000}_{1m;ki} - C^{1000}_{1m;kj}) , \qquad \text{(II.4-36)}$$

$$0 = D^{0000}_{(0)0;k} \qquad \text{(II.4-37)}$$

and

$$0 = \sum_k n_k\left(\sqrt{\frac{c^k_{int}}{k_B}}\,D^{0001}_{(0)0;k} - \sqrt{\frac{2}{3}}\,D^{0010}_{(0)0;k}\right) .$$

(II.4-38)

Recalling equation (II.3-6), the shear viscosity tensor can be written (since $\underline{\underline{B}}_k$ is symmetric and traceless)

$$\underline{\underline{\eta}} = \frac{1}{\sqrt{2}} k_B T \sum_k n_k \ll \underline{\underline{B}}^{(2)}_{k;2000} | \underline{\underline{B}}_k \gg_k . \qquad \text{(II.4-39a)}$$

Expanding in terms of spherical components and then over the total polarization basis yields

$$\underline{\underline{\eta}} = \frac{1}{\sqrt{2}} k_B T \sum_k n_k \sum_{mm'} \ll \underline{\underline{e}}^2_m \, B^{(2)m}_{k;2000} | B^{m'}_k \, \underline{\underline{e}}^2_{m'} \gg$$

$$= \frac{1}{\sqrt{2}} k_B T \sum_k n_k \sum_{mm'} \sum_{pqsta} \underline{\underline{e}}^{2m} \ll B^{(2)m}_{k;2000} | B^{(a)m'}_{k;pqst} \gg B^{pqst}_{(a)m';k} \, \underline{\underline{e}}^2_{m'} .$$

(II.4-39b)

Using the above, the viscosity can be expressed as[8]

$$\underline{\underline{\eta}} = \sum_m \underline{\underline{e}}^{2m} \, \eta_m \, \underline{\underline{e}}^2_m , \qquad \text{(II.4-40)}$$

with

$$\eta_m = \frac{k_B T}{\sqrt{2}} \sum_k n_k \, B^{2000}_{(2)m;k} . \qquad \text{(II.4-41)}$$

Similarly, since D_k is a scalar, equation (II.3-7) for the bulk viscosity tensor can be written

$$\underline{\underline{\kappa}} = \sqrt{2}\, k_B T \sum_k n_k \ll \{ \underline{\underline{B}}^{(2)}_{k;2000} - \frac{\sqrt{3}}{3} B^{(0)}_{k;0010} \underline{\underline{U}} \} | D^{(0)}_k \gg_k$$

$$= \sqrt{2}\, k_B T \sum_k n_k \{ -\frac{\sqrt{3}}{3} \ll B^{(0)}_{k;0010} | D^{(0)}_k \gg_k \underline{\underline{U}} + \sum_m \underline{\underline{e}}^{2m} \ll B^{(2)m}_{k;2000} | D^{(0)}_k \gg_k \}$$

$$= \sqrt{2}\, k_B T \sum_k n_k \{ \underline{\underline{e}}^{20} D^{2000}_{(2)0;k} - \frac{\sqrt{3}}{3} \underline{\underline{U}} \, D^{0010}_{(0)0;k} \} . \qquad \text{(II.4-42)}$$

Consequently, $\underline{\underline{\kappa}}$ can be expressed as

$$\underline{\underline{\kappa}} = \underline{\underline{e}}^{20}\zeta - \underline{\underline{U}}\, \eta_V , \tag{II.4-43}$$

with

$$\zeta = \sqrt{2}\, k_B T \sum_k n_k D^{2000}_{(2)0;k} \tag{II.4-44}$$

and

$$\eta_V = \sqrt{\frac{2}{3}}\, k_B T \sum_k n_k D^{0010}_{(0)0;k} \tag{II.4-45}$$

Recalling equation (II.3-21), the uniform composition thermal conductivity tensor can be written

$$\underline{\underline{\lambda}}_0 = k_B \sum_k \left(\frac{k_B T}{m_k}\right)^{1/2} n_k \ll \{-\sqrt{\frac{5}{2}}\, \underline{\underline{B}}^{(1)}_{k;1010} + \sqrt{\frac{c^k_{int}}{k_B}}\, \underline{\underline{B}}^{(1)}_{k;1001}\} | \underline{A}_k \gg_k . \tag{II.4-46}$$

In terms of spherical components this becomes (after expansion over the total polarization basis)

$$\underline{\underline{\lambda}}_0 = k_B \sum_k \left(\frac{k_B T}{m_k}\right)^{1/2} n_k \sum_{mm'} \sum_{pqsta} \underline{e}^{1m}$$
$$\times \ll \{-\sqrt{\frac{5}{2}}\, B^{(1)m}_{k;1010} + \sqrt{\frac{c^k_{int}}{k_B}}\, B^{(1)m}_{k;1001}\} | B^{(a)m'}_{k;pqst} \gg_k A^{pqst}_{(a)m';k}\, \underline{e}^{1}_{-m'} . \tag{II.4-47}$$

This leads directly to the expression[8]

$$\underset{=}{\lambda}_0 = \sum_m \underset{\sim}{e}^{1m} \lambda_0^m \underset{=}{e}_m^1 , \qquad \text{(II.4-48)}$$

with

$$\lambda_0^m = k_B \sum_k \left(\frac{k_B T}{m_k}\right)^{1/2} n_k \left[\sqrt{\frac{c_{int}^k}{k_B}}\, A^{1001}_{(1)m;k} - \sqrt{\frac{5}{2}}\, A^{1010}_{(1)m;k}\right] . \qquad \text{(II.4-49)}$$

The flow birefringence tensor is treated in direct analogy to $\underset{=}{\eta}$. The spherical components of $\underset{=}{\beta}$ are given by

$$\beta_m = -\pi \sqrt{\frac{2}{15}} \sum_k n_k^2 \left(\alpha_{\parallel} - \alpha_{\perp}\right)_k B^{0200}_{(2)m;k} . \qquad \text{(II.4-50)}$$

The remaining two transport tensors, the multicomponent diffusion tensor, $\underset{=}{D}_{k\ell}$, and the thermal diffusion tensor, $\underset{=}{D}_k^T$, are treated in direct analogy to $\underset{=}{\lambda}_0$. The resulting expressions for the spherical components of $\underset{=}{D}_{k\ell}$ and $\underset{=}{D}_k^T$ are

$$D_{k\ell}^m = \frac{\rho}{n} \frac{n_k}{m_\ell} \left(\frac{k_B T}{m_k}\right)^{1/2} C^{1000}_{(1)m;k\ell} \qquad \text{(II.4-51)}$$

and

$$D_{k;m}^T = (m_k k_B T)^{1/2} n_k A^{1000}_{(1)m;k} . \qquad \text{(II.4-52)}$$

The above expressions for the spherical components of the transport tensors involve specific expansion coefficients, which in turn can be expressed in terms of the $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t \end{Bmatrix}^{(a)}_{k\ell}$, $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t \end{Bmatrix}^{(a)}_{k\ell}$, and $L^{(m)}_{pq}(aa')$ matrix elements, once the set of equations (II.4-31) through (II.4-34) has been solved. In the following section, $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t \end{Bmatrix}^{(a)}_{k\ell}$ and $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{k\ell}$ are examined and related to the collision integrals of Part I. To the extent that these can be determined computationally, the transport properties of a binary gas mixture in the presence of an applied field can now be determined and compared with results obtained experimentally.

II.5 Expansion of the $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$ and $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$ in Terms of the Relative Momentum Collision Integrals

As in Part I, it is possible to expand the scalars, $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$ and $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$, appearing in the matrix equations for the expansion coefficients, in terms of the collision integrals, $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$. Here, to avoid confusion with the k and ℓ indices that appear in the collision integrals, the species of the collision pair are labelled by the indices δ and ν. The development of this section relies heavily upon analogy to Part I, and consequently, avoids details already presented there.

If, as in Part I, only a single component gas is being considered,[8]

$$\left\langle\!\left\langle B^{(a)\alpha}_{pqst} \middle| \mathcal{R} \middle| B^{(a')\alpha'}_{p'q's't} \right\rangle\!\right\rangle = n\left(\frac{\pi\mu}{8k_BT}\right)^{-1/2} \sigma\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)} \delta(a\alpha|a'\alpha') \,. \tag{II.5-1}$$

Recalling that $\mathcal{R}$ can be separated into $\mathcal{R}'$ and $\mathcal{R}''$, this could be rewritten as

$$\left\langle\!\left\langle B^{(a)\alpha}_{pqst} \middle| \mathcal{R} \middle| B^{(a')\alpha'}_{p'q's't} \right\rangle\!\right\rangle$$

$$= n\left(\frac{\pi\mu}{8k_BT}\right)^{-1/2} \delta(a\alpha|a'\alpha')\left\{\sigma'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)} + \sigma''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}\right\}, \tag{II.5-2}$$

in which

$$\sigma'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}(a) = \frac{1}{n}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2}\delta(a\alpha|a'\alpha')\langle\langle B^{(a)\alpha}_{pqst}|\mathcal{R}'|B^{(a')\alpha'}_{p'q's't'}\rangle\rangle$$

(II.5-3)

and

$$\sigma''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}(a) = \frac{1}{n}\left(\frac{\pi\mu}{8k_BT}\right)^{1/2}\delta(a\alpha|a'\alpha')\langle\langle B^{(a)\alpha}_{pqst}|\mathcal{R}''|B^{(a')\alpha'}_{p'q's't'}\rangle\rangle .$$

(II.5-4)

From the development of section I.2 it is also possible to write the above as

$$\sigma'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}(a)$$

$$= (-1)^{q+a+p'}\sum_k (-1)^k\alpha^2(k)\Omega(kq'q)^{1/2}\begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}\sum_{\substack{\ell n \\ \ell' n'}}\Omega(k\ell\ell')^{1/2}$$

$$\times\, I^{(k)}_{\ell n\ell' n';psp's'}\;\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k \qquad \text{(II.5-5)}$$

and

$$\sigma''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}(a)$$

$$= (-1)^{q+a+p'}\sum_k (-1)^k\alpha^2(k)\Omega(kq'q)^{1/2}\begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}\sum_{\substack{\ell n \\ \ell' n'}}\Omega(k\ell\ell')^{1/2}(-1)^{\ell'}$$

$$\times\, I^{(k)}_{\ell n\ell' n';psp's'}\;\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}_k . \qquad \text{(II.5-6)}$$

Equations (II.5-3) and (II.5-4) can be generalized for binary mixtures as follows:

$$\langle B^{(a)\alpha}_{\delta;pqst} | \mathcal{R}'_{\delta\nu} | B^{(a')\alpha'}_{\delta;p'q's't'} \rangle_{\delta} = n_{\nu}\left(\frac{\pi\mu_{\delta\nu}}{8k_BT}\right)^{-1/2} \delta(a\alpha|a'\alpha')\sigma' \begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

(II.5-7)

and

$$\langle B^{(a)\alpha}_{\delta;pqst} | \mathcal{R}''_{\delta\nu} | B^{(a')\alpha'}_{\nu;p'q's't'} \rangle_{\delta} = n_{\nu}\left(\frac{\pi\mu_{\delta\nu}}{8k_BT}\right)^{-1/2} \delta(a\alpha|a'\alpha')\sigma'' \begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}.$$

(II.5-8)

Equations (II.4-29a) and (II.4-29b), along with the above, lead to

$$S' \begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu} = n_{\nu}\left(\frac{\pi\mu_{\delta}}{8k_BT}\right)^{-1/2} \sigma \begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

(II.5-9)

and

$$S'' \begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu} = n_{\nu}\left(\frac{\pi\mu_{\delta\nu}}{8k_BT}\right)^{-1/2} \sigma'' \begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

(II.5-10)

Equations (II.5-5) and (II.5-6) reflect the fact that they have been derived for a single component gas in that they involve the quantities, $I^{(k)}_{\ell n \ell' n';psp's'}$, characteristic of such a system. The generalization of (II.5-5) and (II.5-6) to a binary gas mixture requires use of the Talmi transformation [15]

as presented in Ref. 12. The resultant expressions are

$$\sigma'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

$$= (-1)^{q+a+p'} \sum_k (-1)^k \alpha^2(k)\Omega(kq'q)^{1/2} \begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}$$

$$\times \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2}\, I^{(k)}_{\ell n\ell' n';psp's'}(\alpha_\delta,\alpha_\nu)\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k} \qquad \text{(II.5-11)}$$

and

$$\sigma''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

$$= (-1)^{q+a+p'} \sum_k (-1)^k \alpha^2(k)\Omega(kq'q)^{1/2} \begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix} \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2}$$

$$\times (-1)^{\ell'} \left(\frac{\alpha_\delta}{\alpha_\nu}\right)^{4n'+2\ell'-2s'-p'} I^{(k)}_{\ell n\ell' n';psp's'}(\alpha_\delta,\alpha_\nu)\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}, \qquad \text{(II.5-12)}$$

with $\alpha_\delta = \left(\frac{m_\delta}{2k_BT}\right)^{1/2}$, and $I^{(k)}_{\ell n\ell' n';psp's'}(\alpha_\delta,\alpha_\nu)$ as defined in Ref. 12.

In the above, $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$ are generalizations of the collision integrals given in equations (I.4-15) and (I.6-9) and are similar except that in these quantities, collision partner, a, is of species δ, while b is

of species ν . Thus, the generalization of the single component development of Part I to a binary mixture is accomplished by properly considering the transformation to center of mass and relative coordinates using the Talmi transformation.

Finally,

$$S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

$$= n_\nu\left(\frac{\pi\mu_{\delta\nu}}{8k_BT}\right)^{1/2}(-1)^{q+a+p'}\sum_k (-1)^k\alpha^2(k)\Omega(kqq')^{1/2}\begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}$$

$$\times \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2} I^{(k)}_{\ell n\ell' n';psp's'}(\alpha_\delta,\alpha_\nu)\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$$

(II.5-13)

and

$$S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$$

$$= n_\nu\left(\frac{\pi\mu_{\delta\nu}}{8k_BT}\right)^{1/2}(-1)^{q+a+p'}\sum_k (-1)^k\alpha^2(k)\Omega(kqq')^{1/2}\begin{Bmatrix} q & q' & k \\ p' & p & a \end{Bmatrix}$$

$$\times \sum_{\substack{\ell n \\ \ell' n'}} \Omega(k\ell\ell')^{1/2}(-1)^{\ell'}$$

$$\times \left(\frac{\alpha_\delta}{\alpha_\nu}\right)^{4n'+2\ell'-2s'-p'} I^{(k)}_{\ell n\ell' n';psp's'}(\alpha_\delta,\alpha_\nu)\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k} .$$

(II.5-14)

The above quantities may, in principle, be computed, and consequently, so also the transport properties of a binary gas mixture in an applied field.

II.6 Summary

In summary, the linearized Waldmann-Snider equation is generalized in section II.1 to a binary gas mixture in an applied magnetic field. The detailed nature of this generalization is examined in section II.2, and tensor equations are obtained for the perturbation operators, Φ_k , appearing in the perturbation expansion of the singlet distribution function-density operators, f_k . The expressions for Φ_k are used in section II.3 to obtain tensor equations for the transport properties of a binary gas mixture in an applied field. In section II.4, the tensor equations for the transport properties are transformed into scalar equations involving the quantities $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$ and $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$. And finally, in section II.5, the relative momentum collision integrals of Part I are generalized to collisions involving two molecules of possibly different species. It is then possible to express the scalars, $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$ and $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$, in terms of the binary mixture collision integrals, $\sigma'\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$ and $\sigma''\begin{Bmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{Bmatrix}^{\delta\nu}_{k}$.

With the results of sections II.4 and II.5, it is now possible, in principle, to calculate the scalar quantities, $S'\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$ and $S''\begin{Bmatrix} p & q & s & t \\ p' & q' & s' & t' \end{Bmatrix}^{(a)}_{\delta\nu}$, for a binary mixture and using them, solve a set of matrix equations to

obtain the shear viscosity, bulk viscosity, multi-component diffusion, thermal diffusion, uniform composition thermal conductivity, and flow birefringence of a binary gas mixture in the presence of an applied magnetic field. The field effects on the shear viscosity, thermal conductivity, and flow birefringence are the most widely studied and reported experimentally.[16,17]

The uniform composition thermal conductivity can be related to the experimentally measured thermal conductivity through the Stefan-Maxwell equation.[3,9] To calculate the uniform composition thermal conductivity to the same accuracy as the shear viscosity and flow birefringence requires a larger basis set, due to the greater importance of internal polarizations. Consequently, calculation of the thermal conductivity requires the solution of a larger set of scalar equations than does calculation of either the shear viscosity or flow birefringence.

Calculations of comparable accuracy can be performed for either the shear viscosity or flow birefringence using basis sets of essentially the same size. Since the field effects on the shear viscosity have been widely studied experimentally, the shear viscosity is treated in detail in Part III. The discussion there is intended as an example of the type of treatment that is now possible for any of the transport properties discussed in Part II.

Appendix II.A Demonstration of the Relation Expressed in Equation (II.3-19)

The relation given in (II.3-19) can be demonstrated by means analogous to those used in section 7.4.c of Ref. 9. A sketch of the procedure is given here.

Using (II.2-11)

$$\sum_k \left(\frac{2k_BT}{m_k}\right)^{1/2} \sum_\ell \mathrm{Tr}_k \int f_k^{(0)}\left(W_k^2 + \frac{H'_k}{k_BT} - \frac{5}{2} - \frac{\langle H'_k\rangle_k}{k_BT}\right)\underline{W}_k\, \underline{C}_{k\ell} \cdot \underline{d}_\ell\, d\underline{p}_k \tag{II.A-1a}$$

$$= \sum_{k\ell} \mathrm{Tr}_k \int d\underline{p}_k\, f_k^{(0)} \left[iL_k\underline{A}_k + \sum_{r=1}^{2} (\mathcal{R}'_{kr}\underline{A}_k + \mathcal{R}''_{kr}\underline{A}_r)\right] \underline{C}_{k\ell} \cdot \underline{d}_\ell\, .$$

The RHS of (II.A-1a) can be written

$$= \sum_{k\ell} \mathrm{Tr}_k \int d\underline{p}_k\, f_k^{(0)} \left[\sum_{r=1}^{2} (i\delta_{kr}L_r + \mathcal{R}_{kr})\underline{A}_r \right] \underline{C}_{k\ell} \cdot \underline{d}_\ell\, , \tag{II.A-1b}$$

where $\mathcal{R}_{kr}\underline{A}_r \equiv \mathcal{R}'_{kr}\underline{A}_k + \mathcal{R}''_{kr}\underline{A}_r$. In the above,

$$\mathrm{Tr}_k \int d\underline{p}_k\, f_k^{(0)} [\mathcal{R}_{kr}\underline{A}_r]\underline{C}_{k\ell} \cdot \underline{d}_\ell$$

$$= -(2\pi)^4\hbar^2\, \mathrm{Tr}_k \int d\underline{p}_k\, f_k^{(0)} \{\mathrm{Tr}_r \int d\underline{p}_r\, f_r^{(0)} [\{ \iint d\underline{p}'_r\, d\underline{p}'_k$$

$$\times \langle \mu_{kr}\underline{g}_{kr}|t|\mu_{kr}\underline{g}'_{kr}\rangle(\underline{A}'_k+\underline{A}'_r)\langle \mu_{kr}\underline{g}'_{kr}|\delta(E)t^\dagger|\mu_{kr}\underline{g}_{kr}\rangle\delta(\underline{p}_k+\underline{p}_r-\underline{p}'_k-\underline{p}'_r)\}$$

$$+ \frac{1}{2\pi i}\{\langle \mu_{kr}\underline{g}_{kr}|t|\mu_{kr}\underline{g}_{kr}\rangle(\underline{A}_k+\underline{A}_r) - (\underline{A}_k+\underline{A}_r)\langle \mu_{kr}\underline{g}_{kr}|t^\dagger|\mu_{kr}\underline{g}_{kr}\rangle\}]\}\underline{C}_{k\ell}\cdot\underline{d}_\ell\, , \tag{II.A-2}$$

where the primes on $\mathbf{A}'_k$ and $\mathbf{A}'_r$ indicate a functional dependence on $\mathbf{p}'_k$ and $\mathbf{p}'_r$, respectively.

Switching indices in the term quadratic in t and "symmetrizing",

$$
\begin{aligned}
\mathrm{Tr}_k \int d\mathbf{p}_k\, f_k^{(0)} \mathcal{R}_{kr} \mathbf{A}_r \mathbf{C}_{k\ell} \cdot \mathbf{d}_\ell
&= -(2\pi)^4 \hbar^2\, \mathrm{Tr}_k \mathrm{Tr}_r \iint d\mathbf{p}_k d\mathbf{p}_r \Big\{ \Big[\iint d\mathbf{p}'_r d\mathbf{p}'_k f_k^{(0)'} f_r^{(0)'} \\
&\quad \times \langle \mu_{kr} \mathbf{g}'_{kr} | t^\dagger | \mu_{kr} \mathbf{g}_{kr} \rangle (\mathbf{A}_k + \mathbf{A}_r) \langle \mu_{kr} \mathbf{g}_{kr} | t\,\delta(E) | \mu_{kr} \mathbf{g}'_{kr} \rangle \delta(\mathbf{p}_k + \mathbf{p}_r - \mathbf{p}'_k - \mathbf{p}'_r) \\
&\quad \times \frac{\mathbf{C}'_{k\ell} + \mathbf{C}'_{r\ell}}{2} \Big] \\
&+ \frac{f_k^{(0)} f_r^{(0)}}{2\pi i} \Big[-\frac{\mathbf{C}_{k\ell} + \mathbf{C}_{r\ell}}{2} \langle \mu_{kr} \mathbf{g}_{kr} | t^\dagger | \mu_{kr} \mathbf{g}_{kr} \rangle (\mathbf{A}_k + \mathbf{A}_r) \\
&\quad + (\mathbf{A}_k + \mathbf{A}_r) \langle \mu_{kr} \mathbf{g}_{kr} | t | \mu_{kr} \mathbf{g}_{kr} \rangle \frac{\mathbf{C}_{k\ell} + \mathbf{C}_{r\ell}}{2} \Big] \Big\} \cdot \mathbf{d}_\ell \\
&= -(2\pi)^4 \hbar^2\, \mathrm{Tr}_r \mathrm{Tr}_k \iint d\mathbf{p}_k d\mathbf{p}_r \Big\{ \Big[\iint d\mathbf{p}'_r d\mathbf{p}'_k f_k^{(0)'} f_r^{(0)'} (\mathbf{A}_k + \mathbf{A}_r) \\
&\quad \times \langle \mu_{kr} \mathbf{g}_{kr} | t | \mu_{kr} \mathbf{g}'_{kr} \rangle \frac{\mathbf{C}'_{k\ell} + \mathbf{C}'_{r\ell}}{2} \langle \mu_{kr} \mathbf{g}'_{kr} | \delta(E) t^\dagger | \mu_{kr} \mathbf{g}_{kr} \rangle \\
&\quad \times \delta(\mathbf{p}_k + \mathbf{p}_r - \mathbf{p}'_k - \mathbf{p}'_r) \Big] + \frac{f_k^{(0)} f_r^{(0)}}{2\pi i} \Big[(\mathbf{A}_k + \mathbf{A}_r) \langle \mu_{kr} \mathbf{g}_{kr} | t | \mu_{kr} \mathbf{g}_{kr} \rangle \frac{\mathbf{C}_{k\ell} + \mathbf{C}_{r\ell}}{2} \\
&\quad - \frac{\mathbf{C}_{k\ell} + \mathbf{C}_{r\ell}}{2} \langle \mu_{kr} \mathbf{g}_{kr} | t^\dagger | \mu_{kr} \mathbf{g}_{kr} \rangle (\mathbf{A}_k + \mathbf{A}_r) \Big] \Big\} \cdot \mathbf{d}_\ell , \qquad \text{(II.A-3)}
\end{aligned}
$$

where use has been made of the property[6] that

$$<\mu_{kr}\underline{g}_{kr}|t|\mu_{kr}\underline{g}'_{kr}> \;=\; -<\mu_{kr}\underline{g}'_{kr}|t^{\dagger}|\mu_{kr}\underline{g}_{kr}> . \qquad \text{(II.A-4)}$$

By removing the "symmetrization" from $\underline{A}_k+\underline{A}_r$, and utilizing energy conservation,

$$\mathrm{Tr}_k \int d\underline{p}_k f_k^{(0)}[\mathcal{R}_{kr}\underline{A}_r]\underline{C}_{k\ell}\cdot\underline{d}_\ell \;=\; \mathrm{Tr}_r \int d\underline{p}_r f_r^{(0)}[\mathcal{R}_{rk}\underline{C}_{k\ell}]\underline{A}_r\cdot\underline{d}_\ell \qquad \text{(II.A-5)}$$

It can also be shown by similar but more straightforward means that

$$\mathrm{Tr}_k \int d\underline{p}_k f_k^{(0)}[\delta_{kr}L_r\underline{A}_r]\underline{C}_{k\ell}\cdot\underline{d}_\ell \;=\; \mathrm{Tr}_r \int d\underline{p}_r f_f^{(0)}[\delta_{kr}L_k\underline{C}_{k\ell}]\underline{A}_r\cdot\underline{d}_\ell . \qquad \text{(II.A-6)}$$

Equations (II.A-5) and (II.A-6) allow the demonstration to be completed. Beginning with the RHS of equation (II.A-1),

$$\sum_{k\ell r} \mathrm{Tr}_k \int d\underline{p}_k\; f_k^{(0)}[(i\delta_{kr}L_r+\mathcal{R}_{kr})\underline{A}_r]\underline{C}_{k\ell}\cdot\underline{d}_\ell$$

$$= \sum_{k\ell r} \mathrm{Tr}_r \int d\underline{p}_r\; f_r^{(0)}[(i\delta_{kr}L_k+\mathcal{R}_{rk})\underline{C}_{k\ell}]\underline{A}_r\cdot\underline{d}_\ell . \qquad \text{(II.A-7)}$$

Using (II.2-13) and (II.3-13),

$$\sum_{\ell r} Tr_r \int d\underline{p}_r\, f_r^{(0)} \left[\sum_{k=1}^{2} (i\delta_{kr} L_k + \mathcal{R}_{rk}) \underline{C}_{k\ell} \right] \underline{A}_r \cdot \underline{d}_\ell$$

$$= \sum_{\ell r} Tr_r \int d\underline{p}_r\, f_r^{(0)} \left[iL_r \underline{C}_{r\ell} + \sum_{k=1}^{2} (\mathcal{R}'_{rk} \underline{C}_{r\ell} + \mathcal{R}''_{rk} \underline{C}_{k\ell}) \right] \underline{A}_r \cdot d_\ell$$

$$= \sum_{\ell r} Tr_r \int d\underline{p}_r\, f_r^{(0)} [-\frac{1}{n_r} \underline{V}_r \delta_{r\ell}] \underline{A}_r \cdot \underline{d}_\ell$$

$$= -\sum_\ell \frac{1}{n_\ell m_\ell} \underline{\underline{D}}_\ell^T \cdot \underline{d}_\ell \; . \qquad \text{(II.A-8)}$$

Thus,

$$\sum_k \left(\frac{2k_B T}{m_k}\right)^{1/2} \sum_\ell Tr_k \int f_k^{(0)} (W_k^2 + \frac{H'_k}{k_B T} - \frac{5}{2} - \frac{\langle H'_k \rangle_k}{k_B T}) \underline{W}_k \underline{C}_{k\ell} \cdot \underline{d}_\ell d\underline{p}_k \qquad \text{(II.A-9)}$$

$$= -\sum_\ell \frac{1}{m_\ell n_\ell} \underline{\underline{D}}_\ell^T \cdot \underline{d}_\ell \; ,$$

and the sketch is complete.

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PART II

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PART III.

SHEAR VISCOSITY IN A MAGNETIC FIELD

III.1 Solution of the Transport Equations for a Binary Mixture—Example: The Shear Viscosity

The equations describing the effect of a magnetic field on the transport properties of a binary gaseous mixture, developed in Part II, are valid for mixtures in which both components are diatomic. Since a calculation for a diatom-diatom mixture (or pure diatomic gas) is considerably more difficult than an atom-diatom mixture in which the diatomic species is present in low concentration, the solution of equations (II.4-31) and (II.4-41) for the shear viscosity tensor in this special case is considered in further detail. Thus, the equations of the previous chapter are reduced by considering the limit in which one of the diatomic species becomes spherical while the other diatomic is present in low concentration.

In section III.2 an expression for the shear viscosity is obtained subject to the above restrictions. The truncation of the basis set is that used by Hunter[1] in a discussion of a single component diatomic gas. In section III.3, the collision integrals involved in the shear viscosity calculation are examined in some detail. Their calculation in the classical limit is outlined in section III.4. Finally, a qualitative comparison of the field effects predicted by the expression obtained in section III.2 with experimental observations is discussed in section III.5.

III.2 Spherical Components of the Shear Viscosity Tensor

In this section, expressions for the components of the shear viscosity of a binary mixture in an applied magnetic field are obtained using a truncated basis set. The results are expressed as ratios of determinants. For the special case in which only one component of the gas is diatomic, while the other is atomic, simplifications are possible. Expressions for this special case are given in detail.

Recalling equation (II.4-41), η_m is determined by the expansion coefficients, $B^{2000}_{(2)m;1}$, and $B^{2000}_{(2)m;2}$, where the subscripts, 1 and 2, label the two species present in the binary mixture. If the basis set for each species is truncated to include only the terms $pqst = 2000$ and 0200, (requiring $a = 2$) equation (II.4-31) yields the following set of equations:

$$\sqrt{2} = B^{2000}_{(2)m;1}\left[S'\binom{2000}{2000}^{(2)}_{11} + S''\binom{2000}{2000}^{(2)}_{11} + S'\binom{2000}{2000}^{(2)}_{12}\right] + B^{2000}_{(2)m;2}S''\binom{2000}{2000}^{(2)}_{12}$$

$$+ B^{0200}_{(2)m;1}\left[S'\binom{2000}{0200}^{(2)}_{11} + S''\binom{2000}{0200}^{(2)}_{11} + S'\binom{2000}{0200}^{(2)}_{12}\right] + B^{0200}_{(2)m;2}S''\binom{2000}{0200}^{(2)}_{12}, \tag{III.2-1}$$

$$\sqrt{2} = B^{2000}_{(2)m;1}S''\binom{2000}{2000}^{(2)}_{21} + B^{2000}_{(2)m;2}\left[S'\binom{2000}{2000}^{(2)}_{22} + S''\binom{2000}{2000}^{(2)}_{22} + S'\binom{2000}{2000}^{(2)}_{21}\right]$$

$$+ B^{0200}_{(2)m;1}S''\binom{2000}{0200}^{(2)}_{21} + B^{0200}_{(2)m;2}\left[S'\binom{2000}{0200}^{(2)}_{22} + S''\binom{2000}{0200}^{(2)}_{22} + S'\binom{2000}{0200}^{(2)}_{21}\right], \tag{III.2-2}$$

$$
\begin{aligned}
0 = {} & B^{2000}_{(2)m;1}\left[S'\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{11} + S''\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{11} + S'\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{12}\right] + B^{2000}_{(2)m;2}S''\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{12} \\
& + B^{0200}_{(2)m;1}\left[S'\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{11} + S''\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{11} + S'\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{12} + im(\omega_L)_1\right] \\
& + B^{0200}_{(2)m;2}S''\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{12} \ ,
\end{aligned}
\tag{III.2-3}
$$

and

$$
\begin{aligned}
0 = {} & B^{2000}_{(2)m;1}S''\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{21} + B^{2000}_{(2)m;2}\left[S'\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{22} + S''\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{22} + S'\left(\begin{smallmatrix}0200\\2000\end{smallmatrix}\right)^{(2)}_{21}\right] \\
& + B^{0200}_{(2)m;1}S''\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{21} + B^{0200}_{(2)m;2}\left[S'\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{22} + S''\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{22} + S'\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)^{(2)}_{21}\right. \\
& \left. + im\,(\omega_L)_2\right] \ .
\end{aligned}
\tag{III.2-4}
$$

$B^{2000}_{(2)m;1}$ and $B^{2000}_{(2)m;2}$ can then be expressed as ratios of determinants:

$$
B^{2000}_{(2)m;1} = \frac{\begin{vmatrix} \sqrt{2} & A^{(m)}_{12} & A^{(m)}_{13} & A^{(m)}_{14} \\ \sqrt{2} & A^{(m)}_{22} & A^{(m)}_{23} & A^{(m)}_{24} \\ 0 & A^{(m)}_{32} & A^{(m)}_{33} & A^{(m)}_{34} \\ 0 & A^{(m)}_{42} & A^{(m)}_{43} & A^{(m)}_{44} \end{vmatrix}}{|A^{(m)}_{ij}|} \ , \tag{III.2-5}
$$

and

$$B^{2000}_{(2)m;2} = \frac{\begin{vmatrix} A^{(m)}_{11} & \sqrt{2} & A^{(m)}_{13} & A^{(m)}_{14} \\ A^{(m)}_{21} & \sqrt{2} & A^{(m)}_{23} & A^{(m)}_{24} \\ A^{(m)}_{31} & 0 & A^{(m)}_{33} & A^{(m)}_{34} \\ A^{(m)}_{41} & 0 & A^{(m)}_{43} & A^{(m)}_{44} \end{vmatrix}}{|A^{(m)}_{ij}|} , \qquad \text{(III.2-6)}$$

in which

$$A^{(m)}_{11} = \left[S'\binom{2000}{2000}^{(2)}_{11} + S''\binom{2000}{2000}^{(2)}_{11} + S'\binom{2000}{2000}^{(2)}_{12}\right], \qquad \text{(III.2-7a)}$$

$$A^{(m)}_{12} = S''\binom{2000}{2000}^{(2)}_{12} , \qquad \text{(III.2-7b)}$$

$$A^{(m)}_{13} = \left[S'\binom{2000}{0200}^{(2)}_{11} + S''\binom{2000}{0200}^{(2)}_{11} + S'\binom{2000}{0200}^{(2)}_{12}\right], \qquad \text{(III.2-7c)}$$

$$A^{(m)}_{14} = S''\binom{2000}{0200}^{(2)}_{12} , \qquad \text{(III.2-7d)}$$

$$A^{(m)}_{21} = S''\binom{2000}{2000}^{(2)}_{21} , \qquad \text{(III.2-7e)}$$

$$A^{(m)}_{22} = \left[S'\binom{2000}{2000}^{(2)}_{22} + S''\binom{2000}{2000}^{(2)}_{22} + S'\binom{2000}{2000}^{(2)}_{21}\right] \qquad \text{(III.2-7f)}$$

$$A_{23}^{(m)} = S''\binom{2000}{0200}_{21}^{(2)} , \qquad \text{(III.2-7g)}$$

$$A_{24}^{(m)} = \left[S'\binom{2000}{0200}_{22}^{(2)} + S''\binom{2000}{0200}_{22}^{(2)} + S'\binom{2000}{0200}_{21}^{(2)}\right] , \qquad \text{(III.2-7h)}$$

$$A_{31}^{(m)} = \left[S'\binom{0200}{2000}_{11}^{(2)} + S''\binom{0200}{2000}_{11}^{(2)} + S'\binom{0200}{2000}_{12}^{(2)}\right] , \qquad \text{(III.2-7i)}$$

$$A_{32}^{(m)} = S''\binom{0200}{2000}_{12}^{(2)} , \qquad \text{(III.2-7j)}$$

$$A_{33}^{(m)} = \left[S'\binom{0200}{0200}_{11}^{(2)} + S''\binom{0200}{0200}_{11}^{(2)} + S'\binom{0200}{0200}_{12}^{(2)} + im(\omega_L)_1\right] , \qquad \text{(III.2-7k)}$$

$$A_{34}^{(m)} = S''\binom{0200}{0200}_{12}^{(2)} , \qquad \text{(III.2-7}\ell\text{)}$$

$$A_{41}^{(m)} = S''\binom{0200}{2000}_{21}^{(2)} , \qquad \text{(III.2-7m)}$$

$$A_{42}^{(m)} = \left[S'\binom{0200}{2000}_{22}^{(2)} + S''\binom{0200}{2000}_{22}^{(2)} + S'\binom{0200}{2000}_{21}^{(2)}\right] , \qquad \text{(III.2-7n)}$$

$$A_{43}^{(m)} = S''\binom{0200}{0200}_{21}^{(2)} , \qquad \text{(III.2-7o)}$$

$$A_{44}^{(m)} = \left[S'\binom{0200}{0200}_{22}^{(2)} + S''\binom{0200}{0200}_{22}^{(2)} + S'\binom{0200}{0200}_{21}^{(2)} + im(\omega_L)_2\right] . \qquad \text{(III.2-7p)}$$

Following Ref. 2, η_m can be written as the ratio of determinants:

$$\eta_m = - \frac{\begin{vmatrix} H_{11}^{(m)} & H_{12}^{(m)} & H_{13}^{(m)} & H_{14}^{(m)} & \frac{n_1}{n} \\ H_{21}^{(m)} & H_{22}^{(m)} & H_{23}^{(m)} & H_{24}^{(m)} & \frac{n_2}{n} \\ H_{31}^{(m)} & H_{32}^{(m)} & H_{33}^{(m)} & H_{34}^{(m)} & 0 \\ H_{41}^{(m)} & H_{42}^{(m)} & H_{43}^{(m)} & H_{44}^{(m)} & 0 \\ \frac{n_1}{n} & \frac{n_2}{n} & 0 & 0 & 0 \end{vmatrix}}{|H_{ij}^{(m)}|} \qquad \text{(III.2-8)}$$

in which

$$\begin{aligned} H_{ij}^{(m)} &= \frac{n_1}{k_B T n^2} A_{ij}^{(m)} \qquad \text{for} \quad i=1 \text{ or } 3 \\ &= \frac{n_2}{k_B T n^2} A_{ij}^{(m)} \qquad \text{for} \quad i=2 \text{ or } 4 \end{aligned} \quad . \qquad \text{(III.2-9)}$$

If one of the constituents of the binary mixture is atomic, the term with pqst = 0200 is no longer an allowed member of its basis set, and (III.2-7) no longer applies. For the case in which species 1 is atomic:

$$\eta_m = \frac{\begin{vmatrix} H_{11}^{(m)} & H_{12}^{(m)} & H_{14}^{(m)} & x_1 \\ H_{21}^{(m)} & H_{22}^{(m)} & H_{24}^{(m)} & x_2 \\ H_{41}^{(m)} & H_{42}^{(m)} & H_{44}^{(m)} & 0 \\ x_1 & x_2 & 0 & 0 \end{vmatrix}}{\begin{vmatrix} H_{11}^{(m)} & H_{12}^{(m)} & H_{14}^{(m)} \\ H_{21}^{(m)} & H_{22}^{(m)} & H_{24}^{(m)} \\ H_{41}^{(m)} & H_{42}^{(m)} & H_{44}^{(m)} \end{vmatrix}} , \qquad \text{(III.2-10)}$$

where $x_i = \frac{n_i}{n}$ is the mole fraction of species i .

Letting

$$S\left(\begin{smallmatrix} p \\ p'\end{smallmatrix}, \begin{smallmatrix} q \\ q'\end{smallmatrix}, \begin{smallmatrix} s \\ s'\end{smallmatrix}, \begin{smallmatrix} t \\ t'\end{smallmatrix}\right)_i^{(a)} \equiv \left[S'\left(\begin{smallmatrix} p \\ p'\end{smallmatrix}, \begin{smallmatrix} q \\ q'\end{smallmatrix}, \begin{smallmatrix} s \\ s'\end{smallmatrix}, \begin{smallmatrix} t \\ t'\end{smallmatrix}\right)_{ii}^{(a)} + S''\left(\begin{smallmatrix} p \\ p'\end{smallmatrix}, \begin{smallmatrix} q \\ q'\end{smallmatrix}, \begin{smallmatrix} s \\ s'\end{smallmatrix}, \begin{smallmatrix} t \\ t'\end{smallmatrix}\right)_{ii}^{(a)}\right]$$

$$\equiv n_i\left(\frac{\pi\mu_i}{8k_BT}\right)^{-1/2} \sigma\left(\begin{smallmatrix} p \\ p'\end{smallmatrix}, \begin{smallmatrix} q \\ q'\end{smallmatrix}, \begin{smallmatrix} s \\ s'\end{smallmatrix}, \begin{smallmatrix} t \\ t'\end{smallmatrix}\right)_i^{(a)} , \qquad \text{(III.2-11)}$$

and expanding (III.2-10)

$$\eta_m = \sqrt{\frac{\pi k_BT}{8}} \, [A+Bx_2+Cx_2^2+Dx_2^3]/[E+Fx_2+Gx_2^2+Hx_2^3] , \qquad \text{(III.2-12)}$$

with

$$
\begin{aligned}
A \equiv\ & \left\{\left[\frac{1}{\sqrt{\mu_{21}}}\ \sigma'\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\ \sigma'\binom{0200}{0200}^{(2)}_{21}\right]\right. \\
& - \left[\frac{1}{\sqrt{\mu_{21}}}\ \sigma'\binom{2000}{0200}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\ \sigma'\binom{0200}{2000}^{(2)}_{21}\right] \\
& \left. + \left[\frac{1}{\sqrt{\mu_{21}}}\ \sigma'\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\right]\right\} ,
\end{aligned}
\qquad \text{(III.2-13a)}
$$

$$
\begin{aligned}
B \equiv\ & \left\{\left[\frac{1}{\sqrt{\mu_2}}\sigma\binom{2000}{2000}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\sigma''\binom{2000}{2000}^{(2)}_{12} + \frac{1}{\sqrt{\mu_1}}\sigma\binom{2000}{2000}^{(2)}_{1}\right.\right. \\
& \left. - \frac{1}{\sqrt{\mu_{21}}}\sigma''\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\sigma'\binom{0200}{0200}^{(2)}_{21}\right] - \left[\frac{1}{\sqrt{\mu_{21}}}\sigma\binom{2000}{0200}^{(2)}_{21}\right] \\
& \times \left[\frac{1}{\sqrt{\mu_2}}\sigma\binom{0200}{2000}^{(2)}_{2}\right] - \left[\frac{1}{\sqrt{\mu_2}}\sigma\binom{2000}{0200}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\sigma''\binom{2000}{0200}^{(2)}_{12}\right] \\
& \times \left[\frac{1}{\sqrt{\mu_{21}}}\sigma'\binom{0200}{2000}^{(2)}_{21}\right] + \left[\frac{1}{\sqrt{\mu_{21}}}\sigma'\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_2}}\sigma\binom{0200}{0200}^{(2)}_{2}\right] \\
& + \left[\frac{1}{\sqrt{\mu_{21}}}\sigma''\binom{0200}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\sigma'\binom{2000}{0200}^{(2)}_{21}\right] \\
& + \left[\frac{1}{\sqrt{\mu_2}}\sigma\binom{2000}{2000}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\sigma''\binom{2000}{2000}^{(2)}_{12} + \frac{1}{\sqrt{\mu_1}}\sigma\binom{2000}{2000}^{(2)}_{1}\right. \\
& \left.\left. + \frac{1}{\sqrt{\mu_{21}}}\sigma'\binom{2000}{2000}^{(2)}_{21} - \frac{1}{\sqrt{\mu_{21}}}\sigma''\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\right] - 3A\right\} ,
\end{aligned}
$$

(III.2-13b)

with

$$A \equiv \left\{\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{0200}^{(2)}_{21}\right]\right.$$
$$-\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{2000}^{(2)}_{21}\right]$$
$$\left.+\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\right]\right\}, \qquad \text{(III.2-13a)}$$

$$B \equiv \left\{\left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12} + \frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\right.\right.$$
$$\left.-\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{0200}^{(2)}_{21}\right] - \left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma\binom{2000}{0200}^{(2)}_{21}\right]$$
$$\times\left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{2000}^{(2)}_{2}\right] - \left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\right]$$
$$\times\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{2000}^{(2)}_{21}\right] + \left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{0200}^{(2)}_{2}\right]$$
$$+\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{0200}{2000}^{(2)}_{21}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\right]$$
$$+\left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12} + \frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\right.$$
$$\left.\left.+\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21} - \frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\right]\left[\frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\right] - 3A\right\},$$

(III.2-13b)

$$
\begin{aligned}
C \equiv\ & \Bigg\{\Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12} + \frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1} \\
& - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{0200}^{(2)}_{2}\Bigg] - \Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2} \\
& - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{2000}^{(2)}_{2}\Bigg] + \Bigg[\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Bigg] \\
& \times \Bigg[\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{0200}{0200}^{(2)}_{12}\Bigg] + \Bigg[\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{0200}{2000}^{(2)}_{21}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2} \\
& - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\Bigg] + \Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2} - \frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12} \\
& + \frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1} + \frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12} - \frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Bigg] \\
& \times \Bigg[\frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\Bigg] - 2B - 3A\Bigg\} \qquad \text{(III.2-13c)}
\end{aligned}
$$

$$
\begin{aligned}
D \equiv\ & \Bigg\{\Bigg[\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{0200}^{(2)}_{2} + \frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\Bigg] \\
& - C - B - A\Bigg\}, \qquad \text{(III.2-13d)}
\end{aligned}
$$

$$
\begin{aligned}
E \equiv\ & \Bigg\{\Bigg[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{0200}^{(2)}_{21}\Bigg] \\
& - \Bigg[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{2000}^{(2)}_{21}\Bigg] \\
& + \Bigg[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Bigg]\Bigg[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Bigg]\Bigg[\frac{im}{n}\left(\frac{\pi}{8k_BT}\right)^{1/2}(\omega_L)_2\Bigg]\Bigg\},
\end{aligned}
$$

(III.2-13e)

$$
\begin{aligned}
F \equiv\ & \Big\{\Big[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{0200}^{(2)}_{21}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{1}}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Big\}\Big\{\frac{1}{\sqrt{\mu_{2}}}\,\sigma\binom{2000}{2000}^{(2)}_{2}\Big\} \\
& + \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Big\}\Big] + \Big[\frac{1}{\sqrt{\mu_{1}}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{2}}}\,\sigma\binom{0200}{0200}^{(2)}_{2}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{2}}}\,\sigma\binom{0200}{2000}^{(2)}_{2}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\Big\}\Big] \\
& + \Big[\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{2000}^{(2)}_{21}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Big\} \\
& - \Big\{\frac{1}{\sqrt{\mu_{2}}}\,\sigma\binom{2000}{0200}^{(2)}_{2}\Big\}\Big\{\frac{1}{\sqrt{\mu_{1}}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\}\Big] + \Big[\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{0200}{2000}^{(2)}_{21}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\}\Big] \\
& + \Big[\frac{im}{n}\Big(\frac{\pi}{8k_BT}\Big)^{1/2}(\omega_L)_2\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{1}}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Big\}\Big\{\frac{1}{\sqrt{\mu_{2}}}\,\sigma\binom{2000}{2000}^{(2)}_{2} \\
& + \frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\} + \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\} \\
& - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Big\}\Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Big\}\Big] - 3E\Big\}\ ,
\end{aligned}
$$

(III.2-13f)

$$
\begin{aligned}
G \equiv\ & \Big\{\Big[\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{0200}^{(2)}_{21}\Big\}\Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2}\Big\} \\
& - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{0200}{2000}^{(2)}_{21}\Big\}\Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2}\Big\}\Big] + \Big[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{0200}^{(2)}_{2}\Big] \\
& \times \Big[\Big\{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Big\}\Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2}\Big\} + \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Big\}\Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Big\}\Big] \\
& + \Big[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{2000}^{(2)}_{2}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Big\} \\
& - \Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2}\Big\}\Big\{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{0200}^{(2)}_{21}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\}\Big] + \Big[\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{0200}{2000}^{(2)}_{21}\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2}\Big\} \\
& \times \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Big\} - \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{0200}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2}\Big\}\Big] \\
& \times \Big[\frac{im}{n}\Big(\frac{\pi}{8k_BT}\Big)^{1/2}(\omega_L)_2\Big]\Big[\Big\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2}\Big\}\Big\{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1} \\
& + \frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\} + \Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\Big\}\Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma'\binom{2000}{2000}^{(2)}_{21}\Big\} \\
& - \Big\{\frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}^{(2)}_{21}\Big\}\Big\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma''\binom{2000}{2000}^{(2)}_{12}\Big\}\Big] - 2F - 3E\Big\}\ ,
\end{aligned}
$$

(III.2-13g)

and

$$H \equiv \left\{\left[\left\{\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\right\}\left\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{2000}^{(2)}_{2}\right\}\right]\left[\left\{\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{0200}^{(2)}_{2}\right.\right.\right.$$

$$\left. + \frac{im}{n}\left(\frac{\pi}{8k_B T}\right)^{1/2}(\omega_L)_2\right] - \left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{0200}{2000}^{(2)}_{2}\right]\left[\frac{1}{\sqrt{\mu_2}}\,\sigma\binom{2000}{0200}^{(2)}_{2}\right]$$

$$\left. \times \left[\frac{1}{\sqrt{\mu_{12}}}\,\sigma'\binom{2000}{2000}^{(2)}_{12}\right] - G - F - E\right\} . \qquad \text{(III.2-13h)}$$

Now, for x_2 small, equation (III.2-12) can be expanded in powers of x_2, yielding

$$\eta_m = \sqrt{\frac{\pi k_B T}{8}}\;\frac{A}{E}\left[1 + \left(\frac{B}{A} - \frac{F}{E}\right)x_2 + x_2^2(\ldots.) + \ldots\right] .$$

(III.2-14)

Evaluation of A/E is immediate by inspection:

$$\frac{A}{E} = \left[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1}\right]^{-1} \qquad \text{(III.2-15)}$$

and thus,

$$\eta_m = \sqrt{\frac{\pi\mu_1 k_B T}{8}}\;\frac{1}{\sigma\binom{2000}{2000}^{(2)}_{1}}\left\{1 + \left[\frac{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1} B - F}{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}^{(2)}_{1} A}\right]x_2\right.$$

$$\left. + x_2^2[\;\ldots.\;] + \ldots\right\} . \qquad \text{(III.2-16)}$$

Defining two new quantities,

$$\phi \equiv \frac{(\omega_L)_2}{n} \left(\frac{\pi\mu_{21}}{8k_BT}\right)^{1/2} \frac{\sigma'\binom{2000}{2000}^{(2)}_{21}}{\left[\sigma'\binom{2000}{2000}^{(2)}_{21}\sigma'\binom{0200}{0200}^{(2)}_{21} - \sigma'\binom{2000}{0200}^{(2)}_{21}\sigma'\binom{0200}{2000}^{(2)}_{21}\right]} ,$$

(III.2-17)

and

$$\psi \equiv \frac{(\omega_L)_2}{n} \left(\frac{\pi\mu_{21}}{8k_BT}\right)^{1/2} \left[\sigma'\binom{0200}{0200}^{(2)}_{21}\right]^{-1} , \qquad \text{(III.2-18)}$$

(III.2-16) can be written

$$\eta_m = \eta^{atom} \left\{1 + x_2 \left[\frac{a + b(1 + im\,\psi)}{c(1 + im\,\phi)}\right] + x_2^2\,[\ldots.] + \ldots\right\} \qquad \text{(III.2-19)}$$

in which

$$\eta^{atom} = \sqrt{\frac{\pi\mu_1 k_BT}{8}}\; \frac{1}{\sigma\binom{2000}{2000}^{(2)}_{1}} , \qquad \text{(III.2-20)}$$

$$a = \Big\{\frac{1}{\sqrt{\mu_{12}\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)}\Big[\sigma''\binom{2000}{0200}_{12}^{(2)}\sigma'\binom{0200}{2000}_{21}^{(2)}-\sigma''\binom{0200}{2000}_{21}^{(2)}$$

$$\times\ \sigma'\binom{2000}{0200}_{21}^{(2)}\Big] + \frac{1}{\mu_{12}}\,\sigma'\binom{0200}{2000}_{21}^{(2)}\Big[\sigma'\binom{2000}{0200}_{21}^{(2)}\sigma'\binom{2000}{2000}_{12}^{(2)}$$

$$-\ \sigma''\binom{2000}{0200}_{12}^{(2)}\sigma''\binom{2000}{2000}_{21}^{(2)}\Big] + \frac{1}{\mu_{12}}\,\sigma''\binom{0200}{2000}_{21}^{(2)}$$

$$\times\ \Big[\sigma''\binom{2000}{0200}_{12}^{(2)}\sigma'\binom{2000}{2000}_{21}^{(2)} - \sigma'\binom{2000}{0200}_{21}^{(2)}\sigma''\binom{2000}{2000}_{12}^{(2)}\Big]\Big\}\ , \qquad \text{(III.2-21a)}$$

$$b = \sigma'\binom{0200}{0200}_{21}^{(2)}\Big[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)}\Big\{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)} - \frac{1}{\sqrt{\mu_{12}}}\sigma''\binom{2000}{2000}_{12}^{(2)}$$

$$-\ \frac{1}{\sqrt{\mu_{21}}}\,\sigma''\binom{2000}{2000}_{21}^{(2)}\Big\} + \frac{1}{\mu_{12}}\,\sigma''\binom{2000}{2000}_{12}^{(2)}\sigma''\binom{2000}{2000}_{21}^{(2)}$$

$$-\ \frac{1}{\mu_{12}}\,\sigma'\binom{2000}{2000}_{12}^{(2)}\sigma'\binom{2000}{2000}_{21}^{(2)}\Big]\ , \qquad \text{(III.2-21b)}$$

and

$$c = \frac{\sigma\binom{2000}{2000}_1^{(2)}}{\sqrt{\mu_1\mu_{21}}}\Big[\sigma'\binom{2000}{2000}_{21}^{(2)}\sigma'\binom{0200}{0200}_{21}^{(2)} - \sigma'\binom{2000}{0200}_{21}^{(2)}$$

$$\times\ \sigma'\binom{0200}{2000}_{21}^{(2)}\Big]\ . \qquad \text{(III.2-21c)}$$

For concentrations of the diatomic species sufficiently small, only terms to first order in x_2 need be kept, i.e., only the first two terms in (III.2-19). Under these conditions,

η_m depends only on cross sections for atom-atom and atom-diatom collisions. The primary contribution to η_m is, of course, $\eta^{atom} = \sqrt{\frac{\pi\mu_1 k_B T}{8}} \frac{1}{\sigma\binom{2000}{2000}_1^{(2)}}$. The effects of the field and the corrections due to the presence of the diatomic occur in the term first order in x_2 , with all of the field dependence isolated in the $im\psi$ and $im\phi$ terms.

III.3 Expressions for the Scalars Involved in a Computation of the Shear Viscosity Tensor of an Atom-Diatom Mixture

To calculate the shear viscosity tensor for a small concentration of diatomic species in a predominantly atomic gas, the first two terms of equation (III.2-19) are sufficient. These terms involve ten scalar quantities, one for atom-atom collisions and nine for atom-diatom collisions. Of the nine atom-diatom scalars, five are of the σ' type, while four are of the σ'' variety. The scalar quantities needed for such a calculation are $\sigma\binom{2000}{2000}^{(2)}_{1}$, $\sigma'\binom{2000}{2000}^{(2)}_{21}$, $\sigma'\binom{2000}{2000}^{(2)}_{12}$, $\sigma'\binom{2000}{0200}^{(2)}_{21}$, $\sigma'\binom{0200}{2000}^{(2)}_{21}$, $\sigma'\binom{0200}{0200}^{(2)}_{21}$, $\sigma''\binom{2000}{2000}^{(2)}_{21}$, $\sigma''\binom{2000}{2000}^{(2)}_{12}$, $\sigma''\binom{2000}{0200}^{(2)}_{12}$, $\sigma''\binom{0200}{2000}^{(2)}_{21}$, where once again, 1 is the atomic species and 2 the diatomic.

Equations (II.5-11) and (II.5-12) give expressions for the above quantities in terms of the collision integrals, $\sigma'\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}^{\delta\nu}_{k}$ and $\sigma''\begin{pmatrix} \ell & q & n & t \\ \ell' & q' & n' & t' \end{pmatrix}^{\delta\nu}_{k}$. These expressions involve the quantities, $I^{(k)}_{\ell n\ell' n';psp's'}(\alpha_\delta,\alpha_\nu)$, resulting from the Talmi transformation, six of which are needed for the calculation discussed here:

$$I^{(k)}_{\ell n\ell' n';2020}(\alpha_1,\alpha_1) = \frac{1}{4}\left\{\left[\frac{2\sqrt{15}}{3}\,\delta_{k0} + \sqrt{5}\,\delta_{k1} + \frac{\sqrt{21}}{3}\,\delta_{k2}\right]\delta_{\ell n,10}\delta_{\ell' n',10}\right.$$

$$\left. + \left[\delta_{k0}+\delta_{k1}+\delta_{k2}+\delta_{k3}+\delta_{k4}\right]\delta_{\ell n,20}\delta_{\ell' n',20} + \sqrt{5}\,\delta_{k0}\delta_{\ell n,00}\delta_{\ell' n',00}\right\},$$

(III.3-1a)

$$I^{(k)}_{\ell n\ell' n';2020}(\alpha_1,\alpha_2) = \frac{m_2^2}{(m_1+m_2)^2}\left\{\left[\frac{2\sqrt{15}}{3}\delta_{k0}+\sqrt{5}\,\delta_{k1}+\frac{\sqrt{21}}{3}\delta_{k2}\right]\right.$$

$$\times\left(\frac{m_1}{m_2}\right)\delta_{\ell n,10}\delta_{\ell' n',10}+[\delta_{k0}+\delta_{k1}+\delta_{k2}+\delta_{k3}+\delta_{k4}]\delta_{\ell n,20}\delta_{\ell' n',20}$$

$$\left.+\sqrt{5}\,\delta_{k0}\left(\frac{m_1}{m_2}\right)^2\delta_{\ell n,00}\delta_{\ell' n',00}\right\}, \qquad \text{(III.3-1b)}$$

$$I^{(k)}_{\ell n\ell' n';2020}(\alpha_2,\alpha_1) = \frac{m_1^2}{(m_1+m_2)^2}\left\{\left[\frac{2\sqrt{15}}{3}\delta_{k0}+\sqrt{5}\,\delta_{k1}+\frac{\sqrt{21}}{3}\delta_{k2}\right]\right.$$

$$\times\left(\frac{m_2}{m_1}\right)\delta_{\ell n,10}\delta_{\ell' n',10}+[\delta_{k0}+\delta_{k1}+\delta_{k2}+\delta_{k3}+\delta_{k4}]\delta_{\ell n,20}\delta_{\ell' n',20}$$

$$\left.+\sqrt{5}\,\delta_{k0}\left(\frac{m_2}{m_1}\right)^2\delta_{\ell n,00}\delta_{\ell' n',00}\right\}, \qquad \text{(III.3-1c)}$$

$$I^{(k)}_{\ell n\ell' n';2000}(\alpha_2,\alpha_1) = \frac{m_1}{(m_1+m_2)}\left\{\sqrt{\frac{2}{7}}\,\delta_{k2}\delta_{\ell n,20}\delta_{\ell' n',00}\right\}, \qquad \text{(III.3-1d)}$$

$$I^{(k)}_{\ell n\ell' n';0020}(\alpha_2,\alpha_1) = \frac{m_1}{(m_1+m_2)}\left\{\delta_{k2}\delta_{\ell n,00}\delta_{\ell' n',20}\right\}, \qquad \text{(III.3-1e)}$$

and

$$I^{(k)}_{\ell n\ell' n';0000}(\alpha_2,\alpha_1) = \delta_{k0}\delta_{\ell n,00}\delta_{\ell' n',00}\,. \qquad \text{(III.3-1f)}$$

Using the above and the relation

$$\sigma''\begin{pmatrix}\ell & q & n & t\\ \ell' & o & n' & o\end{pmatrix}^{\delta\nu}_{k} = \sigma'\begin{pmatrix}\ell & q & n & t\\ \ell' & o & n' & o\end{pmatrix}^{\delta\nu}_{k} = \delta_{kq}\sigma'\begin{pmatrix}\ell & q & n & t\\ \ell' & o & n' & o\end{pmatrix}^{\delta\nu}_{k},$$

which requires k be zero if $q=q'=0$, equations (II.5-11) and (II.5-12) can be evaluated for the scalars of interest:

$$\sigma\begin{pmatrix}2000\\2000\end{pmatrix}^{(2)}_{1} = \frac{1}{2}\,\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{11}_{0}, \tag{III.3-2a}$$

$$\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{(2)}_{21} = \frac{m_1^2}{(m_1+m_2)^2}\left\{\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{21}_{0} + 2\left(\frac{m_2}{m_1}\right)\sigma'\begin{pmatrix}1000\\1000\end{pmatrix}^{21}_{0}\right\}, \tag{III.3-2b}$$

$$\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{(2)}_{12} = \frac{m_2^2}{(m_1+m_2)^2}\left\{\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{12}_{0} + 2\left(\frac{m_1}{m_2}\right)\sigma'\begin{pmatrix}1000\\1000\end{pmatrix}^{12}_{0}\right\}, \tag{III.3-2c}$$

$$\sigma'\begin{pmatrix}2000\\0200\end{pmatrix}^{(2)}_{21} = \frac{m_1}{(m_1+m_2)}\,\frac{5\sqrt{14}}{7}\,\sigma'\begin{pmatrix}2000\\0200\end{pmatrix}^{21}_{2}, \tag{III.3-2d}$$

$$\sigma'\begin{pmatrix}0200\\2000\end{pmatrix}^{(2)}_{21} = \frac{m_1}{(m_1+m_2)}\,5\cdot\sigma'\begin{pmatrix}0200\\2000\end{pmatrix}^{21}_{2}, \tag{III.3-2e}$$

$$\sigma'\begin{pmatrix}0200\\0200\end{pmatrix}^{(2)}_{21} = \sigma'\begin{pmatrix}0200\\0200\end{pmatrix}^{21}_{0}, \tag{III.3-2f}$$

$$\sigma''\begin{pmatrix}2000\\2000\end{pmatrix}^{(2)}_{21} = \frac{m_2 m_1}{(m_1+m_2)^2}\left\{\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{21}_{0} - 2\sigma'\begin{pmatrix}1000\\1000\end{pmatrix}^{21}_{0}\right\}, \tag{III.3-2g}$$

$$\sigma''\begin{pmatrix}2000\\2000\end{pmatrix}^{(2)}_{12} = \frac{m_2 m_1}{(m_1+m_2)^2}\left\{\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}^{12}_{0} - 2\sigma'\begin{pmatrix}1000\\1000\end{pmatrix}^{12}_{0}\right\}, \tag{III.3-2h}$$

$$\sigma''\begin{pmatrix}2000\\0200\end{pmatrix}^{(2)}_{21} = \frac{m_1}{(m_1+m_2)}\,\frac{5\sqrt{14}}{7}\,\sigma''\begin{pmatrix}2000\\0200\end{pmatrix}^{21}_{2}, \tag{III.3-2i}$$

and

$$\sigma''\binom{0200}{2000}_{21}^{(2)} = \frac{m_2}{(m_1+m_2)} \cdot 5 \cdot \sigma'\binom{0200}{2000}_{2}^{21} . \qquad \text{(III.3-2j)}$$

In (III.3-2a), (III.3-2b), (III.3-2c), (III.3-2g), and (III.3-2h), use has been made of the fact that

$$\sigma'\binom{0000}{0000}_{0}^{\delta\nu} = \sigma''\binom{0000}{0000}_{0}^{\delta\nu} = 0 . \qquad \text{(III.3-3)}$$

Equations (I.4-15) and (I.6-9) can now be used to obtain expressions for the nine collision integrals appearing in (III.3-2) above.

In general, i.e., if both collision partners are diatomic, equation (I.4-15) yields

$$\sigma'\binom{2000}{2000}_{0}^{\delta\nu} = \frac{4}{15}\frac{\hbar^2\pi}{\mu_{\delta\nu}k_BT}\sum_{\lambda\lambda'}\alpha(\lambda\lambda')\{\delta_{\lambda\lambda'} - (8\pi^2)^{-2}\sum_{j_a'j_b'}[\alpha(\lambda\lambda')(p_{j_a'j_b'})$$

$$\times \begin{pmatrix}\lambda & \lambda' & 2\\ 0 & 0 & 0\end{pmatrix} \int d\gamma\gamma^3 e^{-\gamma^2} \iint dS_a dS_b\, S^*(j_a'j_b'\lambda'|S_aS_b)$$

$$\times \left[(-1)^{-\hbar^{-1}M_3}\begin{pmatrix}\hbar^{-1}\overset{\lambda}{M_3} & -\hbar^{-1}\overset{\lambda'}{M_3} & \overset{2}{0}\end{pmatrix}\right]^* [\gamma^2 - \frac{1}{k_BT}K]\, S(j_a'j_b'\lambda|S_aS_b)]\}_{\delta\nu} .$$

(III.3-4)

If one of the collision partners is spherical, the reduced scattering matrix, $\mathcal{S}$, is independent of the angles associated with the orientation of that collision partner, and the j quantum number associated with rotational states of that collision partner vanishes. Now, utilizing the fact that

$$\mathcal{S}(j_a'j_b'\lambda|S_aS_b) = \exp\left[2iH(j_a'j_b'\lambda|S_aS_b)\right] , \tag{III.3-5}$$

where $H(j_a'j_b'\lambda|S_aS_b)$ is the generalized phase shift introduced by C. F. Curtiss,[3] the $\sigma'\binom{2000}{2000}^{\delta\nu}$ collision integrals appearing in (III.3-2) can be written,

$$\begin{aligned}\sigma'\binom{2000}{2000}_0^{2i} = {} & \frac{4}{15}\frac{\hbar^2\pi}{\mu_{21}k_BT}\sum_{\lambda\lambda'}\alpha(\lambda\lambda')\Big\{\delta_{\lambda\lambda'} - (8\pi^2)^{-1}\sum_{j_a'}\big[\alpha(\lambda\lambda')(p_{j_a'})\\
& \times \begin{pmatrix}\lambda & \lambda' & 2\\ 0 & 0 & 0\end{pmatrix}\int d\gamma\gamma^3 e^{-\gamma^2}\int dS_a \exp[-2iH_{21}^{*}(j_a'\lambda'|S_a)]\\
& \times \left[(-1)^{-\hbar^{-1}M_3^{(a)}}\begin{pmatrix}\lambda & \lambda & 2\\ \hbar^{-1}M_3^{(a)} & -\hbar^{-1}M_3^{(a)} & 0\end{pmatrix}\right]^{*}\\
& \times \left[\gamma^2 - \frac{1}{2I_2k_BT}K^{(a)}\right]\exp\left[2iH_{21}(j_a'\lambda|S_a)\right]\big]\Big\} ,\end{aligned} \tag{III.3-6a}$$

$$\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}_0^{12} = \frac{4}{15}\frac{\hbar^2\pi}{\mu_{12}k_BT}\sum_{\lambda\lambda'}\alpha(\lambda\lambda')\left\{\delta_{\lambda\lambda'} - (8\pi^2)^{-1}\sum_{j_b'}[\alpha(\lambda\lambda')(p_{j_b'})\right.$$

$$\times\begin{pmatrix}\lambda & \lambda' & 2\\0 & 0 & 0\end{pmatrix}\int d\gamma\gamma^3\, e^{-\gamma^2}\int dS_b\, \exp[-2iH_{12}^*(j_b'\lambda'|S_b)]$$

$$\times\left[(-1)^{-\hbar^{-1}M_3^{(b)}}\begin{pmatrix}\lambda & \lambda' & 2\\ \hbar^{-1}M_3^{(b)} & -\hbar^{-1}M_3^{(b)} & 0\end{pmatrix}\right]^*\left[\gamma^2 - \frac{1}{2I_2k_BT}K^{(b)}\right]$$

$$\left.\times\exp[2iH_{12}(j_b'\lambda|S_b)]]\right\}, \tag{III.3-6b}$$

and

$$\sigma'\begin{pmatrix}2000\\2000\end{pmatrix}_0^{11} = \frac{4}{15}\frac{\hbar^2\pi}{\mu_1k_BT}\sum_{\lambda\lambda'}\alpha(\lambda\lambda')\left\{\delta_{\lambda\lambda'} - \left[\alpha(\lambda\lambda')\begin{pmatrix}\lambda & \lambda' & 2\\0 & 0 & 0\end{pmatrix}^2\right.\right.$$

$$\left.\left.\times\int d\gamma\gamma^5\, e^{-\gamma^2}\, e^{2i[H_1(\lambda)-H_1^*(\lambda')]}\right]\right\}. \tag{III.3-6c}$$

The $\sigma'\binom{1000}{1000}_0^{\mu\nu}$ collision integrals are treated in a similar manner to yield

$$\sigma'\binom{1000}{1000}_0^{21} = \frac{2}{3}\frac{\hbar^2\pi}{\mu_{21}k_BT}\sum_{\lambda\lambda'}\alpha(\lambda\lambda')\left\{\frac{1}{2}\delta_{\lambda\lambda'} - (8\pi^2)^{-1}\sum_{j_a'}[\alpha(\lambda\lambda')(p_{j_a'})\right.$$

$$\times\begin{pmatrix}\lambda & \lambda' & 1\\ 0 & 0 & 0\end{pmatrix}\int d\gamma\gamma^2\, e^{-\gamma^2}\int dS_a\, \exp[-2iH_{21}^*(j_a'\lambda'|S_a)]$$

$$\times\left[(-1)^{-\hbar^{-1}M_3^{(a)}}\begin{pmatrix}\lambda & \lambda' & 1\\ \hbar^{-1}M_3^{(a)} & -\hbar^{-1}M_3^{(a)} & 0\end{pmatrix}\right]^*$$

$$\left.\times\left[(\gamma^2 - \frac{1}{2I_2k_BT}K^{(a)})^{1/2}\right]\exp[2iH_{21}(j_a'\lambda|S_a)]\right]\Bigg\} \qquad \text{(III.3-7a)}$$

and

$$\sigma'\binom{1000}{1000}_0^{12} = \frac{2}{3}\frac{\hbar^2\pi}{\mu_{12}k_BT}\sum_{\lambda\lambda'}\alpha(\lambda\lambda')\left\{\frac{1}{2}\delta_{\lambda\lambda'} - (8\pi^2)^{-1}\sum_{j_b'}[\alpha(\lambda\lambda')(p_{j_b'})\right.$$

$$\times\begin{pmatrix}\lambda & \lambda' & 1\\ 0 & 0 & 0\end{pmatrix}\int d\gamma\gamma^2\, e^{-\gamma^2}\int dS_b\, \exp[-2iH_{12}^*(j_b'\lambda'|S_b)]$$

$$\times\left[(-1)^{-\hbar^{-1}M_3^{(b)}}\begin{pmatrix}\lambda & \lambda' & 1\\ \hbar^{-1}M_3^{(b)} & -\hbar^{-1}M_3^{(b)} & 0\end{pmatrix}\right]^*$$

$$\left.\times\left[(\gamma^2 - \frac{1}{2I_2k_BT}K^{(b)})^{1/2}\right]\exp[2iH_{12}(j_b'\lambda'|S_b)]\right]\Bigg\} . \qquad \text{(III.3-7b)}$$

The remaining collision integrals appearing in (III.3-2) are treated individually and yield somewhat more complicated expressions than those of (III.3-6) and (III.3-7).

Using equations (I.4-15) and (I.6-9), $\sigma'\binom{2000}{0200}_2^{21}$ and $\sigma''\binom{2000}{0200}_2^{12}$ can be written

$$
\begin{aligned}
\sigma'\binom{2000}{0200}_2^{21} = & -\frac{2\sqrt{3}}{75}\frac{\hbar^2\pi}{\mu_{21}k_BT} \times (8\pi^2)^{-1} \sum_{j_a'\lambda}{}' \Big\{\alpha(j_a')(p_{j_a'}) \\
& \times ([\underline{\underline{J}}]^{(2)}:[\underline{\underline{J}}]^{(2)})^{1/2}_{j_a'} R_0^{(2)}(\epsilon_{j_a'})\alpha^2(\lambda) \\
& \times \sum_{\alpha=-2}^{2} (i)^{\alpha} \int d\gamma\gamma^3 e^{-\gamma^2} \int dS_a \exp[-2iH_{21}^{*}(j_a'\lambda|S_a)]D_{\alpha 0}^2(S_a) \\
& \times (-1)^{j_a'-\hbar^{-1}L_3^{(a)}} \begin{pmatrix} 2 & j_a' & j_a' \\ -\alpha & \hbar^{-1}L_3^{(a)}+\alpha & -\hbar^{-1}L_3^{(a)} \end{pmatrix} \\
& \times \left[\gamma^2 - \frac{1}{2I_2k_BT} K^{(a)}\right] \exp[2iH_{21}(j_a'\lambda|S_a)]\Big\} , \qquad \text{(III.3-8a)}
\end{aligned}
$$

and

$$
\begin{aligned}
\sigma''\binom{2000}{0200}_2^{12} = & -\frac{2\sqrt{3}}{75}\frac{\hbar^2\pi}{\mu_{12}k_BT} \times (8\pi^2)^{-1} \sum_{j_b'\lambda} \Big\{\alpha(j_b')(p_{j_b'}) \\
& \times ([\underline{\underline{J}}]^{(2)}:[\underline{\underline{J}}]^{(2)})^{1/2}_{j_b'} R_0^{(2)}(\epsilon_{j_b'})\alpha^2(\lambda) \\
& \times \sum_{\alpha=-2}^{2} (i)^{-\alpha} \int d\gamma\gamma^3 e^{-\gamma^2} \int dS_b \exp[-2iH_{12}^{*}(j_b'\lambda|S_b)] \\
& \times (-1)^{j_b'-\hbar^{-1}L_3^{(b)}} \begin{pmatrix} 2 & j_b' & j_b' \\ \alpha & \hbar^{-1}L_3^{(b)}-\alpha & -\hbar^{-1}L_3^{(b)} \end{pmatrix} D_{\alpha 0}^2(S_b) \\
& \times \left[\gamma^2 - \frac{1}{2I_2k_BT} K^{(b)}\right] \exp[2iH_{12}(j_b'\lambda|S_b)]\Big\} , \qquad \text{(III.3-8b)}
\end{aligned}
$$

while $\sigma'\binom{0200}{2000}^{21}_{2}$ and $\sigma'\binom{0200}{0200}^{21}_{0}$ become

$$\sigma'\binom{0200}{2000}^{21}_{2} = -\frac{2\sqrt{3}}{75}\frac{\hbar^2\pi}{\mu_{21}k_BT} \times (8\pi^2)^{-1} \sum_{j_a'\lambda\lambda'} \left\{(p_{j_a'})\alpha^2(\lambda\lambda')\right.$$

$$\times \sum_{\alpha=-2}^{2}\sum_{\beta=-2}^{2} (i)^{\alpha+\beta} \begin{pmatrix}\lambda & \lambda' & 2\\ 0 & 0 & 0\end{pmatrix} \int d\gamma\gamma\, e^{-\gamma^2} \int dS_a \exp[-2iH_{21}^*(j_a'\lambda'|S_a)$$

$$\times I_a(2,-\alpha)D^2_{\alpha\beta}(S_a) \left[(-1)^{-\hbar^{-1}M_3^{(a)}}\begin{pmatrix}\lambda & \lambda' & 2\\ \hbar^{-1}M_3^{(a)} & -\hbar^{-1}M_3^{(a)}+\beta & -\beta\end{pmatrix}\right]^*$$

$$\left.\times \left[R_0^{(2)}(\epsilon_{j_a'} + \frac{1}{2I_2k_BT}K^{(a)})\right] \exp[2iH_{21}(j_a'\lambda|S_a)]\right\}, \quad \text{(III.3-8c)}$$

and

$$\sigma'\binom{0200}{0200}^{21}_{0} = \frac{1}{5}\frac{\hbar^2\pi}{\mu_{21}k_BT}\left\{\left[\frac{5}{2}\sum_{\lambda}\alpha^2(\lambda)\right] - (8\pi^2)^{-1}\right.$$

$$\times \sum_{j_a'\lambda}\left[\alpha(j_a')(p_{j_a'})([\underline{\underline{J}}]^{(2)}:[\underline{\underline{J}}]^{(2)})^{1/2}_{j_a'}\, R_0^{(2)}(\epsilon_{j_a'})\alpha^2(\lambda) \sum_{\alpha\alpha'\beta}(-1)^{\beta}(i)^{\alpha+\alpha'}\right.$$

$$\times \int d\gamma\gamma\, e^{-\gamma^2} \int dS_a \exp[-2iH_{21}^*(j_a'\lambda|S_a)]$$

$$\times D^2_{\alpha',-\beta}(S_a)(-1)^{j_a'-\hbar^{-1}L_3^{(a)}} \begin{pmatrix}2 & j_a' & j_a'\\ -\alpha' & \hbar^{-1}L_3^{(a)}+\alpha' & -\hbar^{-1}L_3^{(a)}\end{pmatrix}$$

$$\times I_a(2,-\alpha)D^2_{\alpha\beta}(S_a)\left[R_0^{(2)}(\epsilon_{j_a'} + \frac{1}{2I_2k_BT}K^{(a)})\right]$$

$$\left.\times \exp[2iH_{21}(j_a'\lambda|S_a)]\right\}. \quad \text{(III.3-8d)}$$

From equations (III.3-6a) and (III.3-6b) and equations (III.3-7a) and (III.3-7b) it is apparent that

$$\sigma'\binom{2000}{2000}^{21}_{0} = \sigma'\binom{2000}{2000}^{12}_{0} \qquad \text{(III.3-9)}$$

and

$$\sigma'\binom{1000}{1000}^{21}_{0} = \sigma'\binom{1000}{1000}^{12}_{0} . \qquad \text{(III.3-10)}$$

Thus, seven collision integrals need be evaluated to obtain the five spherical components of the viscosity tensor for an atom-diatom mixture subject to an applied field. In the next section, these collision integrals, $\sigma'\binom{2000}{2000}^{11}_{0}$, $\sigma'\binom{2000}{2000}^{21}_{0}$, $\sigma'\binom{1000}{1000}^{21}_{0}$, $\sigma'\binom{2000}{0200}^{21}_{2}$, $\sigma''\binom{2000}{0200}^{12}_{2}$, $\sigma'\binom{0200}{2000}^{21}_{2}$, and $\sigma'\binom{0200}{0200}^{21}_{0}$, are written in forms appropriate for computational purposes.

III.4 Classical Limit Expressions for the Collision Integrals

Expressions for the classical limits of the seven collision integrals listed at the end of section III.3 are next considered. The procedure for obtaining such classical limits is discussed in detail in the work of K. Squire [5] and R. Wood, [4] and consequently, is only sketched here.

An expression of the form

$$\iint dS_a dS_b \; e^{-2iH^*(j_a j_b \lambda' | S_a S_b)} \, A \, e^{2iH(j_a j_b \lambda | S_a S_b)} \, ,$$

where A is any operator in the space of the six Euler angles indicated by S_a and S_b, may be rewritten as

$$\iint dS_a dS_b \; e^{-2iH^*(j_a j_b \lambda | S_a S_b)} e^{2i[H^*(j_a j_b \lambda | S_a S_b) - H^*(j_a j_b \lambda' | S_a S_b)]}$$

$$\times \; A \, e^{2iH(j_a j_b \lambda | S_a S_b)} \tag{III.4-1}$$

It is shown in Ref. 5 that there exists a unitary operator, $P(\lambda; S_a S_b)$, such that

$$e^{2iH(j_a j_b \lambda | S_a S_b)} = P(\lambda; S_a S_b) \, e^{2i\eta_\lambda} \, , \tag{III.4-2}$$

where η_λ is the spherical phase shift. This makes it possible to write (III.4-1) as

$$\iint dS_a dS_b\, P^{-1}(\lambda;S_aS_b)e^{2i[H^*(j_aj_b\lambda|S_aS_b)-H^*(j_aj_b\lambda'|S_aS_b)]}$$

$$\times\ A\, P(\lambda;S_aS_b) \;=\; \iint dS_a dS_b\; e^{-i\xi\chi_\xi(j_aj_b\lambda|S_aS_b)}\,\tilde{A}\ , \tag{III.4-3}$$

in which $\tilde{A} = P^{-1}(\lambda;S_aS_b)\,A\,P(\lambda;S_aS_b)$; $\xi = \lambda'-\lambda$; and the generalized angle of deflection, $\chi_\xi(j_aj_b\lambda|S_aS_b)$, is defined such that

$$-\frac{1}{2}\xi\chi_\xi(j_aj_b\lambda|S_aS_b) \equiv P^{-1}(\lambda;S_aS_b)[H^*(j_aj_b\lambda|S_aS_b)-H^*(j_aj_b\lambda+\xi|S_aS_b)]$$

$$\times\ P(\lambda;S_aS_b)\ , \tag{III.4-4}$$

and consequently,

$$P^{-1}(\lambda;S_aS_b)e^{2i[H^*(j_aj_b\lambda|S_aS_b)-H^*(j_aj_b\lambda+\xi|S_aS_b)]}\,P(\lambda;S_aS_b)$$

$$=\ e^{-i\xi\chi_\xi(j_aj_b\lambda|S_aS_b)} \tag{III.4-5}$$

Next, the operator, $\tilde{A}$, is replaced by the classical limit, $A(S_aS_b)$, which is a function,[5] and χ_ξ is replaced by its limit, which is a function independent of ξ . Finally, infinite sums over discrete indices are replaced by corresponding integrals over continuous variables. Details of the above procedure are discussed in Ref. 5.

Carrying out the above, the classical limits of $\sigma'\left({2000 \atop 2000}\right)_0^{11}$, $\sigma'\left({2000 \atop 2000}\right)_0^{21}$, and $\sigma'\left({1000 \atop 1000}\right)_0^{21}$ are given by the following expressions:

$$\sigma'\left({2000 \atop 2000}\right)_0^{11} \xrightarrow[\text{Limit}]{\text{Classical}} \frac{8\pi}{5} \int bdb \int d\gamma \gamma^7 e^{-\gamma^2} \sin^2\chi_1 \, , \qquad \text{(III.4-6a)}$$

$$\sigma'\left({2000 \atop 2000}\right)_0^{21} \xrightarrow[\text{Limit}]{\text{Classical}} \frac{2}{5\pi} \int d\epsilon_{rot} e^{-\epsilon_{rot}} \int dS_a \int bdb \int d\gamma \gamma^5 e^{-\gamma^2}$$

$$\times \left[\gamma^2 - \frac{1}{2I_2 k_B T} K^{(a)}\right] \left[\sin^2\chi_{21}(S_a) + \frac{M_3^{(a)2}}{2\mu_{12} k_B T \gamma^2} \frac{1}{b^2} \cos^2\chi_{21}(S_a)\right] , \qquad \text{(III.4-6b)}$$

$$\sigma'\left({1000 \atop 1000}\right)_0^{21} \xrightarrow[\text{Limit}]{\text{Classical}} \frac{4\pi}{3} \int d\gamma e^{-\gamma^2} \int bdb \left\{\gamma^5 - 2\gamma^4 \int d\epsilon_{rot} e^{-\epsilon_{rot}}\right.$$

$$\times (8\pi^2)^{-1} \int dS_a \left[\gamma^2 - \frac{1}{2I_2 k_B T} K^{(a)}\right]^{1/2}$$

$$\times \left.\left[1 - \frac{M_3^{(a)2}}{2\mu_{12} k_B T \gamma^2} \frac{1}{b^2}\right]^{1/2} \cos\chi_{21}(S_a)\right\} , \qquad \text{(III.4-6c)}$$

in which b is the classical impact parameter,[6] ϵ_{rot} is the dimensionless rotational energy[6] of the diatomic molecule, χ_1 is the spherical angle of deflection for colliding atoms, $\chi_{21}(S_a)$ is the generalized angle of deflection for an atom-diatom collision, and $M_3^{(a)}$ and $K^{(a)}$ are functions defined in Ref. 5.

The classical limits of $\sigma'(^{2000}_{0200})^{21}_{2}$, $\sigma''(^{2000}_{0200})^{12}_{2}$, $\sigma'(^{0200}_{2000})^{21}_{2}$, and $\sigma'(^{0200}_{0200})^{21}_{0}$ are somewhat more difficult to obtain. They are found by replacing $M_3^{(a)*}$ by $M_3^{(a)}$, $L_3^{(a)}$ by $L_3^{(a)}$, $K^{(a)}$ by $K^{(a)}$, $I_a(2,-\alpha)$ by $I^{(a)}(2,-\alpha)$, and $D^2_{\alpha\beta}(S_a)$ by $\bar{D}^2_{\alpha\beta}(S_a)$, and again introducing the generalized angle of deflection. The quantities $M_3^{(a)}$, $L_3^{(a)}$, and $K^{(a)}$ are those of References 4 and 5, while $I^{(a)}(2,-\alpha)$ and $\bar{D}^2_{\alpha\beta}(S_a)$ are the classical limits of $P^{-1}I_a(2,-\alpha)P$ and $P^{-1}D^2_{\alpha\beta}(S_a)P$, respectively. The classical limits of the $R_0^{(2)}$ Wang Chang-Uhlenbeck polynomials are independent of the arguments. They are $[\frac{4}{3}(\frac{2I_2k_BT}{\hbar^2})^2 - \frac{1}{2}(\frac{2I_2k_BT}{\hbar^2})]$, while $([\underline{J}]^{(2)}:[\underline{J}]^{(2)})_{ja}$ is $\frac{1}{6}j_a(j_a+1)[4j_a(j_a+1)-3]$. Following Reference 5 and utilizing the above, the classical limits of $\sigma'(^{2000}_{0200})^{21}_{2}$, $\sigma''(^{2000}_{0200})^{12}_{2}$, $\sigma'(^{0200}_{2000})^{21}_{2}$, and $\sigma'(^{0200}_{0200})^{21}_{1}$ may be obtained.

Once the classical limits of the seven collision integrals discussed in this section have been obtained, it becomes possible to compute them numerically. The methods used by R. Wood for a Lennard-Jones 6-12 potential with P_2 anisotropic attractive and repulsive terms may be extended in a straightforward manner to the collision integrals involved in a calculation of the shear viscosity tensor of an atom-diatom system subjected to an applied magnetic field. Though straightforward, the computations indicated here are expected to be quite lengthy.

It is possible, however, to discuss the nature of the effect of an applied field on the viscosity tensor obtained in section III.2 without carrying out such a calculation. This is discussed in the following section.

III.5 Relationship of η_m to Previously Calculated and Experimentally Measured Results

In this section, attention is focussed on the qualitative behavior of η_m as given by equation (III.2-19). Both low and high magnetic field limits are examined, as well as the spherical limit and the experimentally measureable quantities. Qualitatively, η_m is shown to be consistent with recent computations [4] of η in the absence of a field, and with the measurements of Beenakker and others [7] of viscosities of gases with diamagnetic diatomic components in the presence of an applied magnetic field.

Recalling equations (III.2-19) and (III.2-20),

$$\eta_m \cong \eta^{atom} \{1 + x_2[\frac{a+b\{1+im\psi\}}{c\{1+im\phi\}}]\} , \qquad \text{(III.5-1)}$$

with

$$\eta^{atom} = (\frac{\pi\mu_1 k_B T}{8})^{1/2} \frac{1}{\sigma\binom{2000}{2000}_1^{(2)}} , \qquad \text{(III.5-2)}$$

and in which only terms to first order in the mole fraction of the diatomic species have been kept.

In the limit that the magnetic field, H_M , goes to zero, ψ and ϕ go to zero, and

$$\eta_m \xrightarrow{H_M \to 0} \eta_0 \qquad \text{(III.5-3)}$$

with

$$\eta_0 = \eta^{atom} \{1 + x_2 \frac{a+b}{c}\} \qquad \text{(III.5-4)}$$

If expanded in orders of the anisotropy of the atom-diatom potential, the zeroth and first order terms of η_0 are, respectively,

$$\begin{aligned}\eta_0(0) = \eta^{atom}\{1+x_2 & \left[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)}\left\{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)}\right.\right. \\ & - \frac{1}{\sqrt{\mu_{12}}}\,\sigma_0''\binom{2000}{2000}_{12}^{(2)} - \frac{1}{\sqrt{\mu_{21}}}\,\sigma_0''\binom{2000}{2000}_{21}^{(2)}\Big\} \\ & \left. + \frac{1}{\mu_{12}}\,\sigma_0''\binom{2000}{2000}_{21}^{(2)}\sigma_0''\binom{2000}{2000}_{12}^{(2)} - \frac{1}{\mu_{12}}\,\sigma_0'\binom{2000}{2000}_{12}^{(2)}\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right] \\ & \times \left[\frac{1}{\sqrt{\mu_1\mu_{21}}}\,\sigma\binom{2000}{2000}_1^{(2)}\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right]^{-1}\} \qquad \text{(III.5-5)}\end{aligned}$$

and

$$\eta_0(1) = 0 . \qquad \text{(III.5-6)}$$

In the above, the collision integrals subscripted with zeros are the contribution to the collision integral from the spherical portion of the interaction potential, i.e., the zeroth order in the anisotropy contribution. Through first order in the

anisotropy, η_0 is identical to η computed by R. Wood.[4] (See Appendix III.A.) The second and higher order contributions are expected to differ slightly due to the somewhat different truncation procedure. (See section III.2.)

In the spherical limit, i.e., the limit in which only terms to zeroth order in the anisotropy of the potential are kept, $\phi_{\text{spherical}} \to \psi_{\text{spherical}}$, $a \to 0$, and $\eta_m(0)$ becomes independent of both the field and the index m. This is as expected, since the field effects are due to the non-sphericity of the interaction potential.

In the large field limit, η_m again becomes independent of the field. For $m = 0$, of course, it is identical to the low field limit. However, for $m \neq 0$

$$\eta_m \xrightarrow{H_M \to \infty} \eta^{\text{atom}} \{1 + x_2 \frac{b\psi}{c\phi}\} . \qquad \text{(III.5-7)}$$

Since all field dependence is isolated in ψ and ϕ, (III.5-7) can be written (ψ and ϕ are both proportional to $\frac{(\omega_L)_2}{n}$, which is proportional to H_M/p)

$$\eta_{m\neq 0}(H_M \to \infty) \to \eta^{\text{atom}} \{1 + x_2 \frac{\sqrt{\mu_1 \mu_{21}}\ b}{\sigma\binom{2000}{2000}_1^{(2)} \sigma'\binom{2000}{2000}_{21}^{(2)} \sigma'\binom{0200}{0200}_{21}^{(2)}}\} , \qquad \text{(III.5-8)}$$

which is clearly independent of field. $\eta_{m\neq 0}(H_M\to\infty)$ is identical to $\eta_0(0)$ if the zero subscripts are removed from the atom-diatom collision integrals occurring in $\eta_0(0)$. The fact that $\eta_{m\neq 0}(H_M\to\infty)$ is independent of the field is explained physically by the fact that the precession frequency becomes much greater than the collision frequency, resulting in a statistical averaging [8] of the diatomic species for large field. The net result is a saturation of the Senftleben-Beenakker effect and is observed experimentally. [7,8]

Turning to experimental results, the quantities that have been measured [7,8] are the changes in $\frac{i}{3}(\eta_2-\eta_{-2})$, $\frac{i}{3}(\eta_1-\eta_{-1})$, and $\frac{1}{6}(\eta_2+\eta_{-2}+\eta_1+\eta_{-1})$ induced by an applied magnetic field. The first two quantities are

$$\frac{i}{3}(\eta_2-\eta_{-2}) = \frac{4}{3}\,\eta^{\text{atom}}\,x_2\,\frac{(a+b)\phi-b\psi}{c[1+4\phi^2]} \qquad \text{(III.5-9a)}$$

and

$$\frac{i}{3}(\eta_1-\eta_{-1}) = \frac{2}{3}\,\eta^{\text{atom}}\,x_2\,\frac{(a+b)\phi-b\psi}{c[1+\phi^2]} \qquad \text{(III.5-9b)}$$

The interesting point to note here is that since both ψ and ϕ are directly proportional to H_M/p , the above quantities are odd with respect to the field. This is observed experimentally. [8]

The third quantity, measured by Beenakker and co-workers,[8,9] is (to first order in x_2)

$$-\frac{\Delta\eta}{\eta} = \left\{\frac{4\eta_0-(\eta_2+\eta_{-2}+\eta_1+\eta_{-1})}{4\eta_0}\right\} \cong \frac{x_2}{2}\left\{\frac{[5+8\phi^2][(a+b)\phi^2-b\psi\phi]}{c[1+5\phi^2+4\phi^4]}\right\} \tag{III.5-10}$$

This expression is even in the field, as is observed experimentally. Furthermore, in the low field limit, $\frac{\Delta\eta}{\eta}$ is proportional to the square of H_M/p , while in the high field limit, it becomes constant:

$$-\frac{\Delta\eta}{\eta} \xrightarrow{H_M \to \infty} x_2\left\{\frac{(a+b)}{c} - \frac{\sqrt{\mu_1\mu_{21}}\ b}{\sigma\left(\begin{smallmatrix}2000\\2000\end{smallmatrix}\right)_1^{(2)}\sigma'\left(\begin{smallmatrix}2000\\2000\end{smallmatrix}\right)_{21}^{(2)}\sigma'\left(\begin{smallmatrix}0200\\0200\end{smallmatrix}\right)_{21}^{(2)}}\right\} . \tag{III.5-11}$$

$(-\frac{\Delta\eta}{\eta})$ grows monotonically from zero to the above saturation limit. All of these characteristics are consistent with experimental observations.

It is interesting to note that since both the high and low field limits are independent of m , except for $m = 0$,

$$\left(-\frac{\Delta\eta}{\eta}\right) \xrightarrow{H_M \to \infty} \frac{\eta_m(H_M \to 0) - \eta_{m\neq 0}(H_M \to \infty)}{\eta_m(H_M \to 0)} . \tag{III.5-12}$$

Thus, the saturation value for the relative change in the $m = \pm 2, \pm 1$ spherical components of the viscosity tensor is identical to the value measured for the mixture in the experimental apparatus of Beenakker and co-workers.

The important result of this section is that using the minimum basis capable of exhibiting field effects, it has been possible to obtain expressions for the spherical components of the viscosity tensor which behave qualitatively in a manner that is consistent with experimentally observed behavior. Since, in principle, computations of the field effects are no more difficult than the recent non-field calculations of R. Wood, it is now possible to obtain theoretical values for the field effects on the viscosity of gaseous mixtures that contain small concentrations of diatomic molecules in a predominantly atomic gas. There is considerable experimental information with which these theoretical results can be compared.

III.6 Summary

To summarize, in section III.2 an expression (equation (III.2-19)) is obtained for the spherical components of the shear viscosity tensor of an atom-diatom mixture in the presence of an applied magnetic field. This expression is shown in section III.5 to be qualitatively consistent with experimental observations of these field effects. A calculation using equation (III.2-19) requires the consideration of ten scalars,

$$\sigma\binom{2000}{2000}^{(2)}_{1},\ \sigma'\binom{2000}{2000}^{(2)}_{21},\ \sigma'\binom{2000}{2000}^{(2)}_{12},\ \sigma'\binom{2000}{0200}^{(2)}_{21},\ \sigma'\binom{0200}{2000}^{(2)}_{21},$$

$$\sigma'\binom{0200}{0200}^{(2)}_{21},\ \sigma''\binom{2000}{2000}^{(2)}_{21},\ \sigma''\binom{2000}{2000}^{(2)}_{12},\ \sigma''\binom{2000}{0200}^{(2)}_{12},\ \text{and}$$

$$\sigma''\binom{0200}{2000}^{(2)}_{21},$$

which, under closer examination in section III.3, prove to require the evaluation of seven collision integrals,

$$\sigma'\binom{2000}{2000}^{11}_{0},\ \sigma'\binom{2000}{2000}^{21}_{0},\ \sigma'\binom{1000}{1000}^{21}_{0},\ \sigma'\binom{2000}{0200}^{21}_{2},$$

$$\sigma'\binom{0200}{2000}^{21}_{2},\ \text{and}\ \sigma''\binom{2000}{0200}^{12}_{2}.$$

A computation similar to that recently completed by R. Wood [4] requires expressions for the classical limits of the above collision integrals. The procedure for obtaining such classical limit expressions for the collision integrals examined in section III.3 is outlined in section III.4. It relies heavily upon the work of K. Squire, [5] and the reader is referred to that work for a more detailed treatment.

The fact that equation (III.2-19) is consistent with the available experimental results is most satisfying. It can also be shown that the classical limit expression for $\sigma'\binom{2000}{2000}_0^{11}$ leads to an expression for η^{atom} that is consistent with those of other treatments. The RHS of *(III.4-6a)* is equivalent to $\frac{8\pi}{5}\sqrt{\frac{\mu_1}{2\pi k_B T}}\,\Omega_{11}^{(2,2)}$ where $\Omega_{11}^{(2,2)}$ is an omega integral defined in Reference 2 and equivalent to the $\Omega_{11}^{(\ell)}(s)$ of Chapman and <u>Cowling</u>. [10] Using this result and the fact that $\eta^{atom} = \sqrt{\frac{\pi\mu_1 k_B T}{8}}\,\frac{1}{\sigma\binom{2000}{2000}_1^{(2)}}$, the classical limit expression for η^{atom} becomes

$$\eta_{Cl}^{atom} = \frac{5}{8}\,\frac{k_B T}{\Omega_{11}^{(2,2)}}\,, \qquad \text{(III.6-1)}$$

which is precisely the expression given in Ref. 2.

Thus, the dominant contribution to the shear viscosity tensor is consistent with other theoretical developments, while the qualitative behavior is consistent with experimental observations. It remains to be seen if a numerical calculation will lead to results that are numerically close to those obtained by experiment.

Appendix III.A Demonstration of the Equivalence of $\eta_0(0)$ and $\eta^{WOOD}(0)$

Since there are no contributions to η_0 and η^{WOOD} that are first order in the anisotropy, η_0 and η^{WOOD} are identical through first order in the anisotropy if $\eta_0(0)$ and $\eta^{WOOD}(0)$ are the same. Equation (III.5-5) can be written

$$\eta_0(0) = \eta_{CL}^{atom}\,[1 + x_2\tilde{\eta}_1(0)]\ , \qquad \text{(III.A-1)}$$

where $\eta_{CL}^{atom} = \frac{5}{8}\frac{k_B T}{\Omega_{11}^{(2,2)}}$ is identical to η_0^{WOOD}, and

$$\tilde{\eta}_1(0) = \left[\left\{\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)} - \frac{1}{\sqrt{\mu_{12}}}\left[\sigma_0''\binom{2000}{2000}_{12}^{(2)} + \sigma_0''\binom{2000}{2000}_{21}^{(2)}\right]\right\}\right.$$

$$+ \left\{\frac{1}{\mu_{12}}\left[\sigma_0''\binom{2000}{2000}_{21}^{(2)}\,\sigma_0''\binom{2000}{2000}_{12}^{(2)} - \sigma_0'\binom{2000}{2000}_{12}^{(2)}\,\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right]\right.$$

$$\left.\left.\times\left[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)}\right]^{-1}\right\}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right]^{-1} \qquad \text{(III.A-2)}$$

Now,

$$\sigma\binom{2000}{2000}_1^{(2)} = \frac{1}{2}\,\sigma'\binom{2000}{2000}_0^{11} \xrightarrow[\text{Limit}]{\text{Classical}} \frac{4\pi}{5}\sqrt{\frac{\mu_1}{2\pi k_B T}}\;\Omega_{11}^{(2,2)}\ ,$$

(III.A-3a)

$$\sigma_0''\binom{2000}{2000}_{12}^{(2)} = \frac{m_1 m_2}{(m_1+m_2)^2}\left\{\sigma_0'\binom{2000}{2000}_0^{12} - 2\sigma_0'\binom{1000}{1000}_0^{12}\right\}$$

$$\xrightarrow[\text{Limit}]{\text{Classical}} \frac{m_1 m_2}{(m_1+m_2)^2}\sqrt{\frac{\pi\mu_{12}}{2k_BT}}\left\{\frac{8}{5}\,\Omega_{12}^{(2,2)}(0) - \frac{16}{3}\,\Omega_{12}^{(1,1)}(0)\right\},$$

(III.A-3b)

$$\sigma_0''\binom{2000}{2000}_{12}^{(2)} = \xrightarrow[\text{Limit}]{\text{Classical}} \sigma_0''\binom{2000}{2000}_{12}^{(2)}$$

$$\sigma_0'\binom{2000}{2000}_{12}^{(2)} = \frac{m_2^2}{(m_1+m_2)^2}\left\{\sigma_0'\binom{2000}{2000}_0^{12} + 2\left(\frac{m_1}{m_2}\right)\sigma_0'\binom{1000}{1000}_0^{12}\right\}$$

$$\xrightarrow[\text{Limit}]{\text{Classical}} \frac{m_2^2}{(m_1+m_2)^2}\sqrt{\frac{\pi\mu_{12}}{2k_BT}}\left\{\frac{8}{5}\,\Omega_{12}^{(2,2)}(0)\right.$$

$$\left. + \frac{16}{3}\left(\frac{m_1}{m_2}\right)\Omega_{12}^{(1,1)}(0)\right\}, \qquad \text{(III.A-3c)}$$

and

$$\sigma_0'\binom{2000}{2000}_{21}^{(2)} = \frac{m_1^2}{(m_1+m_2)^2}\left\{\sigma_0'\binom{2000}{2000}_0^{21} + 2\left(\frac{m_2}{m_1}\right)\sigma_0'\binom{1000}{1000}_0^{21}\right\}$$

$$\xrightarrow[\text{Limit}]{\text{Classical}} \frac{m_1^2}{(m_1+m_2)^2}\sqrt{\frac{\pi\mu_{12}}{2k_BT}}\left\{\frac{8}{5}\,\Omega_{12}^{(2,2)}(0)\right.$$

$$\left. + \frac{16}{3}\left(\frac{m_2}{m_1}\right)\Omega_{12}^{(1,1)}(0)\right\}. \qquad \text{(III.A-3d)}$$

Using equation (3.2-5) of Ref. 2,

$$\left\{\frac{1}{\mu_{12}}\left[\sigma_0''\binom{2000}{2000}_{21}^{(2)}\sigma_0'\binom{2000}{2000}_{12}^{(2)} - \sigma_0'\binom{2000}{2000}_{12}^{(2)}\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right]\right\}$$

$$\times\left\{\left[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right]\right\}^{-1}$$

$$= \frac{-\frac{2}{3}\frac{M}{m_1}\sqrt{\mu_1\mu_{12}}\left(\frac{\sigma_{12}^2}{\sigma_{11}^2}\right)\Omega_{12}^{(2,2)^*}(0)\;\Omega_{12}^{(1,1)^*}(0)}{\Omega_{11}^{(2,2)^*}\;\left\{\frac{m_1}{5}\,\Omega_{12}^{(2,2)^*}(0) + \frac{m_2}{3}\,\Omega_{12}^{(1,1)^*}(0)\right\}}\,, \qquad \text{(III.A-4a)}$$

where $M \equiv (m_1+m_2)$, and

$$\left[\frac{1}{\sqrt{\mu_1}}\,\sigma\binom{2000}{2000}_1^{(2)} - \frac{2}{\sqrt{\mu_{12}}}\,\sigma_0''\binom{2000}{2000}_{12}^{(2)}\right]\left[\frac{1}{\sqrt{\mu_{21}}}\,\sigma_0'\binom{2000}{2000}_{21}^{(2)}\right]^{-1}$$

$$= \frac{\left\{\frac{1}{10}\frac{m_2 M}{\sqrt{\mu_1\mu_{12}}}\left(\frac{\sigma_{11}^2}{\sigma_{12}^2}\right)\Omega_{11}^{(2,2)^*} + 2m_2\left[\frac{1}{5}\,\Omega_{12}^{(2,2)^*} - \frac{1}{3}\,\Omega_{12}^{(1,1)^*}\right]\right\}}{\left\{\frac{m_1}{5}\,\Omega_{12}^{(2,2)^*} + \frac{m_2}{3}\,\Omega_{12}^{(1,1)^*}\right\}}\,.$$

(III.A-4b)

Equations (III.A-4a) and (III.A-4b) can be added to yield

$$\tilde{\eta}_1(0) = \left\{m_2[H_1(0)+2H_2(0)] - [H_3(0)H_4(0) - m_1m_2H_2(0)^2]\,[m_1H_1(0)]^{-1}\right\}$$

$$\times\;\{H_3(0)\}^{-1}\,, \qquad \text{(III.A-5)}$$

where the $H_i(0)$ are the spherical limits of the H_i quantities defined[4] by R. Wood.

Finally,

$$\tilde{\eta}_1(0) = \tilde{\eta}_1^{WOOD}(0) , \qquad \text{(III.A-6)}$$

and consequently,

$$\eta_0(0) = \eta^{WOOD}(0) . \qquad \text{(III.A-7)}$$

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CONCLUSION

In Part I, the collision integrals, developed by Hunter and Snider[1] and essential to Hunter's treatment of a single component diatomic gas in an applied field,[2] are expressed in terms of the reduced scattering matrix of Curtiss[3] and co-workers. The introduction of several operators leads to considerable simplification of the expressions for the collision integrals. The intent of this work is to move closer to calculations of the transport properties of dilute diatomic gases in applied fields. Recognizing the difficulties inherent in carrying out a calculation which requires treatment of diatom-diatom interactions leads to the aim of first discussing a physical situation which requires only the consideration of atom-atom and atom-diatom interactions. This leads to the development in Part II of expressions for the transport properties of binary gaseous mixtures in applied fields.

Part II is an extension of Hunter's work on single component gases[2] to binary mixtures. As in Hunter's work, scalar equations for the shear viscosity and thermal conductivity tensors are obtained. In addition, scalar equations are obtained for the bulk viscosity, multi-component and thermal diffusion, and flow birefringence tensors of binary mixtures in applied fields. The motive for discussing mixtures is the desire to treat systems composed of a diatomic species in low concentration in a

predominantly atomic gas. Such systems require the treatment of atom-diatom and atom-atom interactions only in a calculation of the transport properties. The shear viscosity of such a system in an applied field is examined in detail in Part III.

An expression for the shear viscosity of an atom-diatom mixture is obtained in Part III. As mentioned in the summary, the expression obtained is consistent with both experimental results[4] and the numerical treatment of such systems in the absence of a field recently completed by R. Wood.[5] Treatments of single component systems and at least one treatment of binary mixtures[6] have also yielded results in qualitative agreement with experiment. This, however, is the first treatment of mixtures using techniques[2] which require no truncations prior to the tensor analyses.

A sketch is also given in Part III of a procedure which can lead to the eventual calculation of the collision integrals occurring in the expression for the shear viscosity. A large amount of work, however, must yet be done in applying the numerical methods[5] of R. Wood to a calculation of the shear viscosity of an atom-diatom mixture in an applied magnetic field. This leads to a consideration of possible future work related to the present development.

Clearly, the next step in this development is the actual calculation of the transport properties of dilute gases in applied fields. The calculation that seems most immediately feasible is

that of the shear viscosity of atom-diatom mixtures in an applied magnetic field. Other transport properties of atom-diatom mixtures are possible once the scalar equations of Part II have been solved in analogy with the shear viscosity development of Part III.

Calculation of the transport properties of single component diatomic gases in applied fields requires considerably more complex computer programs than those needed for the atom-diatom mixtures. In principle, however, these are also possible. Part I is a step in that direction.

The Senftleben-Beenakker effect is felt to be a potentially sensitive probe[7] of intermolecular potentials. Its use as such, however, is limited at present by the relatively small amount of theoretical work[4] in this area. The present need is for calculations to go along with the considerable experimental information already available. This thesis is an attempt to bridge some of the gap between experimental evidence and theoretical understanding of the Senftleben-Beenakker effect.

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